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The Cholesteric Domain Texture

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Abstract—When a large pitch cholesteric is held between parallel glass plates a distance d apart, near the isotropic transition, a characteristic striped pattern appears. The distance between stripes is about the half pitch $p_{00}/2$ (providing $d > p_{00}$) and the texture has no measurable optical rotatory power. It does not appear if $d \ll p_{00}$.

Assuming that the molecules lie in planes perpendicular to the glass plates and twist uniformly in the interior of the sample about an axis parallel to the glass plates, we have solved the Frank equation(1) when tangential (or homoeotropic) boundary conditions are applied. The solution predicts a lattice of $\chi^{(2)}$ disclinations at the surface of the sample, the distance between the χ's being related to the half-pitch. We have found that this configuration is not stable within a distance $p_0/4$ ($d \sim p_0$) of the disclination and we suggest that this results in the splitting of the χ into a λ and a τ.(2) This latter configuration appears to adequately explain the experimentally observed features of the cholesteric domain texture.

The same type of instability occurs when a χ is parallel to the cholesteric axis, and leads also to a splitting into a λ and τ. A complete calculation is presented for this case.

1. Introduction

We present a possible interpretation of the domain texture shown by the cholesteric–nematic mixture *p-n*-methoxybenzylidene-butylaniline (MBBA) and cholesterol propionate near the cholesteric–isotropic transition.(3) Specifically we observe a series of dark and bright lines appear (see for example Fig. 1) when the cholesteric phase is allowed to form slowly between parallel glass plates by evaporation of a solvent (toluene). This solvent has been added to the normally thermotropic MBBA for the purpose of rendering it isotropic. The cholesteric texture formed in this manner has a remarkably orderly appearance and very often consists of a parallel array of stripes all more or less pointing towards the isotropic region in the middle of the sample.

This texture disappears by jarring the sample and turns to the more stable cholesteric homogeneous texture (twist axis perpendicular to glass plates). It does not form readily if the thickness of the sample, d, is about or smaller than the equilibrium pitch $|p_{00}|$.† In fact, when $d \ll |p_{00}|$, quite different textures have been observed. The pitch, p_0, refers to the pitch as deduced from measuring the distance between stripes. When the pitch p_{00} is measured by using the Cano Wedge(4) technique, we find $|p_0| > |p_{00}|$.

The role of the solvent is non-negligible. With no solvent present, merely mixing MBBA with suitable amounts of a cholesteric compound to obtain a given pitch (see Appendix A) and then heating the sample to near T_c, the isotropic–mesophase transition does not result in exactly the same optical contrast as when the solvent is present. In the former case, the stripes are blurry and the contrast of the different regions of the texture is quite poor.

Raising the lowering the focus over a sample, such as shown in Fig. 1, very often results in a displacement of the bright line laterally. This appears to be particularly true when the thickness of the sample $d \sim |p_0|$. The direction of the displacement can be in either sense, that is, if we are in focus over a series of parallel lines such as shown in Fig. 1, when raising the focus, we see that either the whole pattern shifts either to the right or to the left, or, only, some of the lines shift to the right whereas others shift to the left.

Now, let us assume (naively) that the stripes in Fig. 1 arise because we have a perfect cholesteric without any kind of singularity of the orientation of the molecules, whose axis of twist lies parallel to the glass plates but perpendicular to the stripes. The banded appearance then arises because we have a periodic change in the refractive index of the medium when the direction of polarization is parallel to the bands. But, then for light vibrating at right angles to the bands, this idea leads to a constant refractive index in the medium and consequently, the banded appearance should disappear if the polarizer alone is used to view the sample. In fact, the observed

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† The pitch $p = 2\pi/q$ is positive for a right-hand cholesteric and negative for a left-hand cholesteric, by convention. In order not to create confusion, we use the notation $|p|$ when referring to the value of the pitch.

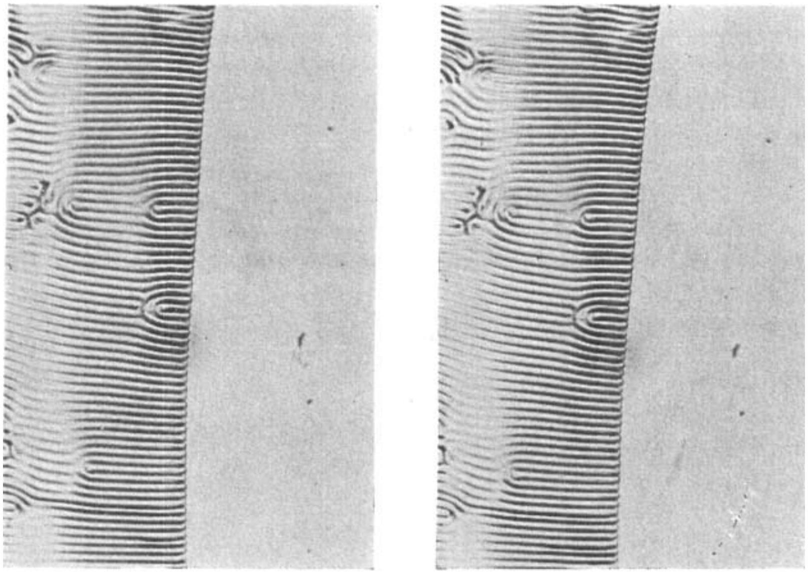
contrast seems to depend very little on the orientation of the sample above the polarizer as we show in Fig. 1(a) and 1(b).

As a first step towards understanding the above we have studied the solutions which minimize the Frank free energy equation

$$F = \tfrac{1}{2}K_{11}(\operatorname{div}\mathbf{n})^2 + K_{22}(\mathbf{n}\cdot\operatorname{curl}\mathbf{n}+q_0)^2 + K_{33}(\mathbf{n}\,\Lambda\,\operatorname{curl}\mathbf{n})^2 \qquad (1)$$

for the case of a cholesteric confined between parallel glass plates, the twist axis being parallel to the plates and the molecules subjected to given constraints at the boundary (strong anchoring). We present the results of this calculation in the next section. In the third section, we suggest modifications to this naive model to explain the above optical observations. All the calculations are done assuming

$$K_{11} = K_{22} = K_{33}.$$



(a) (b)

Figure 1. Sample with polarizer alone: (a) direction of vibration of incident light parallel to stripes. We imagine the molecules to be placed so that their long axis is parallel to the plane defined by a stripe and a line perpendicular to the plane of the page. They turn in this plane; (b) direction of vibration of incident light perpendicular to stripes. Very little difference is seen between Fig. 1 (a) and (b). Pitch here is about 12 μ. Sample thickness $d \sim 20\ \mu$.

2. Naive Model

(A) CALCULATION

We propose a model of variable pitch $p(x,z) = 2\pi/q(x,z)$ whereby a large pitch cholesteric may be able to pass from a twisted configuration inside the sample (i.e. far from the boundary) to an essentially *nematic* (tangential $\theta = n\pi$ or homoeotropic $\theta = n\pi/2$ n = odd integer) orientation at the boundary. The pitch is variable in the sense that it is a function of position, however,

$$\int_{-p_0/2}^{p_0/2} q(x,z)\,\mathrm{d}x = 2\pi. \tag{2}$$

Our coordinates are shown in Fig. 2. The angle $\theta = q(x,z)\,x$ is between the director **n** and the $x-y$ plane. Our assumed configuration is

$$\begin{aligned} n_x &= 0 \\ n_y &= \cos q(x,z)x \\ n_z &= \sin q(x,z)x \end{aligned} \tag{3}$$

the middle of the sample is $z = 0$, when $z = \pm d/2$, $\theta(x, \pm d/2) = 0$. The free energy density is then

$$\mathrm{F} = \frac{K}{2}\left[x^2\left(\frac{\partial q}{\partial z}\right)^2 + \left(q_{00} - x\frac{\partial q}{\partial x} - q\right)^2\right] + F_0 \tag{4}$$

where K is the isotropic elastic constant and $q_{00} = 2\pi/p_{00}$ is the

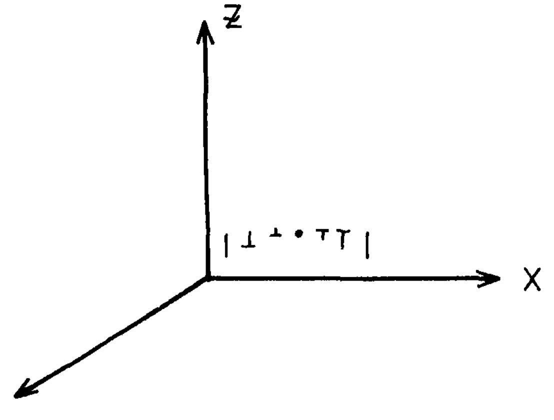


Figure 2. Coordinates for variable pitch calculation. The molecular configuration is indicated along the x-axis following the notation of Kléman and Friedel.[2]

equilibrium pitch. We require that when $q(x,z) = q_{00}$, $F - F_0 = 0$, so we minimize (4) with respect to $q(x,z) - q_{00} = q'$ to obtain

$$x^2\frac{\partial^2 q'}{\partial z^2} + x^2\frac{\partial^2 q'}{\partial x^2} + 2x\frac{\partial q'}{\partial x} = 0. \tag{5}$$

Taking into account the symmetry of the problem, the solution to Eq. (5) is

$$q'(x,z) = \frac{1}{x}\sum\nolimits_m A_m \cosh mz \sin mx + (q_0 - q_{00})$$

or

$$\theta = q_0 x + \sum\nolimits_m A_m \cosh mz \sin mx = \theta_0 + \delta\theta \tag{6}$$

where m^2 is the separation constant of (5). Requiring that $\delta\theta(x,z) = \delta\theta(x + p_0/2,\ z)$ implies $m = 2nq_0$ where n is an integer. The interval over which we can solve (6) is then $-p_0/4 < x < p_0/4$, $-d/2 < z < d/2$. The tangential condition $\theta(x,\ \pm d/2) = 0$ yields

$$\theta = q_0 x + \sum_{n=1} \frac{(-)^n}{n}\frac{\cosh 2nq_0 z}{\cosh nq_0 d}\sin 2nq_0 x. \tag{7}$$

In the homoeotropic case we have only to add $\pi/2$ to (7).

We note that the series appearing in (7) has for an upper limit the series $\sum_n (1/n)\exp - 2\,|\,q_0\,|(|\,z\,| - d/2)n$, which is absolutely converging for any value of x and z, except $z = \pm d/2$. For $x = \pm p/4$, θ jumps by an angle of π, as plotted in Fig. 3, when $z = \pm d/2$, but does not show any discontinuity for any other value of z. We are

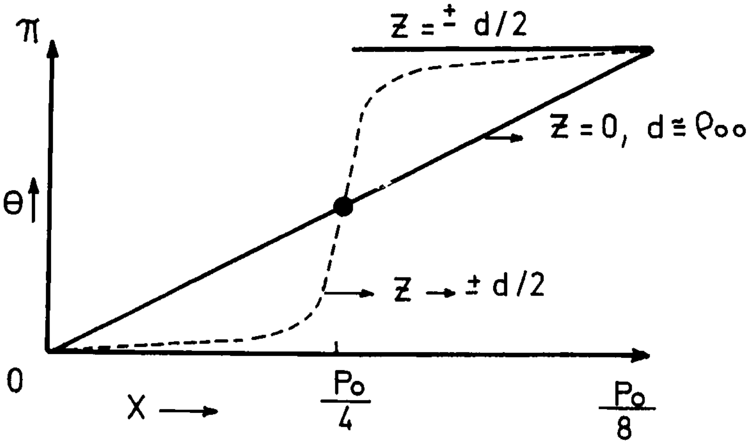


Figure 3. θ as a function of x for different values of z. When $z = \pm d/2$, θ jumps discontinuously by π, however, is continuous for all $z \neq \pm d/2$, $x \neq p_0/4$.

then describing a situation in which χ (see Appendix C) disclinations$^{(2)}$ of strength $\frac{1}{2}$ are periodically distributed on both sides of the specimen, on the boundaries (cf. Fig. 4). The repartition of the director n in the vicinity of the singular point is very similar to that already suggested by de Gennes$^{(5)}$ for the different problem of the Grandjean Cano-Wedge.

From (7), we integrate over the period with respect to x, we get the energy for a layer at thickness z, of length $|p_0|/2$.

$$\mathscr{F}(z) = \frac{K}{2}\left[\frac{|p_0|}{2}(q_{00}-q_0)^2 + q_0^2\,|p_0| \sum_{n=1} \frac{\cosh 4nq_0 z}{\cosh^2 nq_0 d}\right]. \tag{8}$$

It is easy to show that providing $z \neq \pm d/2$ an upper bound for Eq. (8) exists and we are allowed to integrate term by term to yield for the total energy (per unit length along the y axis)

$$\mathscr{F}_C = \frac{\pi K}{2}\left[\frac{(q_{00}-q_0)^2}{|q_0|}(d-a) + z\sum_n \frac{\sinh nq_0(d-a)\cosh nq_0(d-a)}{n\cosh^2 nq_0 d}\right] \tag{9}$$

where a is the radius of the singular region reputedly a few molecular lengths.

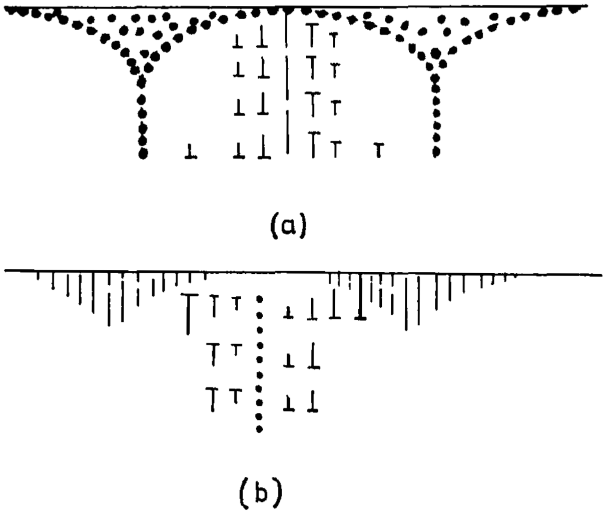


Figure 4. Repartition of the director **n** in the vicinity of a χ disclination located at the surface in the case of (a) tangential boundary conditions (b) homoeotropic conditions.

Let $\mathscr{F}_N$ be the energy of a cholesteric of pitch $2\pi/q_{00}$ aligned as a nematic. Then

$$\mathscr{F}_N = \frac{K}{2}\frac{|p_0|}{2} q_{00}^2 \tag{10}$$

for an equivalent volume requiring $\mathscr{F}_C < \mathscr{F}_N$ yields the condition

$$|p_0| > |p_{00}|/2. \tag{11}$$

An upper limit for the energy density[8] yields

$$F(z) < \frac{K}{2}\left[\frac{|p_0|}{2}(q_{00}-q_0)^2 + \frac{1}{2|p_0|}\frac{\exp -|q_0|(d-2|z|)}{\sinh|q_0|(d-2z)}\right] \tag{12}$$

which gives us an upper bound for the total energy of a half period

$$\mathscr{F}_C < \frac{\pi K}{2}\left[\frac{(q_0-q_{00})^2}{|q_0|}(d-2a) + \ln\frac{1}{4|q_0|a} + \text{core energy}\right] \tag{13}$$

$(\pi K/2)\ln 1/(4|q_0|a)$ is the energy of a lattice of χ disclinations with average separation q_0^{-1}. Minimizing (13) with respect to q_0, we find

$$-\ln 4|q_0|a = 2(|q_{00}| - |q_0|)d \tag{14}$$

which gives the dependence of $|q_0|$ on d.

(B) DISCUSSION

The above model provides an explanation for most of the observations. Essentially, it foresees (a) the existence of singularities of the molecular configuration, regularly spaced and hereabove described as χ disclinations, (b) a dependence of the observed pitch on the thickness of the sample. Its central assumption, i.e. that the molecules lie in planes, is however very crude, and we shall see that it does not hold in the vicinity of the disclination.

Let us first consider the variation of the energy with the thickness. Inserting Eq. (14) in Eq. (15) yields

$$\mathscr{F}_C < \frac{\pi K}{2}\left[\frac{(q_0-q_{00})^2}{|q_0|}(d-2a) + 2d\,|q_{00}-q_0| + \text{core energy}\right]. \tag{15}$$

The energy is then reduced to the core energy when the periodicity is equal to half the pitch. As a consequence, the texture is preferentially tilted with respect to the plate when the thickness is not large enough to allow q_0 to approach q_{00} according to Eq. (14) (cf. Fig. 5). This latter supposition is supported by the fact that the bright regions occasionally are displaced sideways upon raising the focus. Also (cf. Table 1) the measured pitch $|p_0|$ is always somewhat bigger

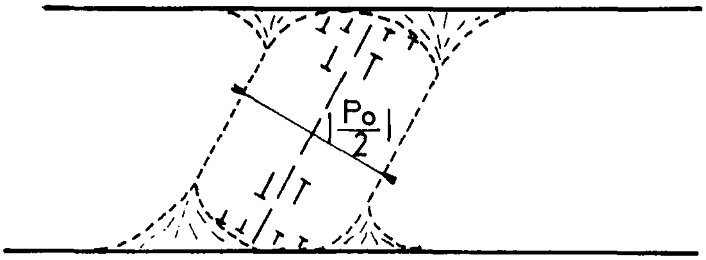


Figure 5. Tilting of the domain texture with respect to the plate.

than $| p_{00} |$ as measured by the Cano Wedge technique. Observations made independently of ours[6] confirm the tilting of the texture.

When the angle of tilt increases, the interaction energies between disclinations are not so well balanced as calculated in Eq. (15), and the dissymetry between the " image " disclinations does not allow for a continuously increasing tilt. Also notice that, following Eq. (7), $\partial\theta/\partial x$ is not uniform in the center of the specimen ($z = 0$) when $d \ll | p_{00} |$. For d small enough, other situations than the cholesteric domain texture may then be more favourable. Specifically, we have grown the cholesteric texture in a wedge from an isotropic (lyotropic) phase. The thickness of the wedge varied from about 1 mm at the wide end to about 2 μ. The surface of the wedge had been rubbed as à la Chatelain.[7] We observed that the striped texture formed

TABLE 1 Comparison of Equilibrium Pitch, p_{00} with Pitch Observed in Striped Texture (p_0). Theoretically, we expect $p_0 > p_{00}/2$ and a thickness dependence, $p_0(d)$ following Eq. (14). The error in these measurements precludes the possibility of drawing any conclusion concerning a possible thickness dependence (see text)

d	Half pitch in microns		
(in microns)	I	II	III
Cano Wedge ($p_{00}/2$)	6.17 ±0.10	5.97 ±0.13 Sample I (24 hours later)	4.4 ±0.2
($p_0/2$)			
18 μ	6.2 ±0.6	9.75 ±1	
36 μ	7.8 ±0.6	7.4 ±0.5	5.1 ±0.3
50 μ	7.9 ±0.5		5.3 ±0.3
75 μ	8.4 ±1	8.3 ±1.0	6.58 ±0.8

quite easily, even at the thickest end with very little change in the periodicity of the stripes as a function of thickness until a thickness between p_0 and $p_0/2$. At this thickness, a rather abrupt transformation to an oriented nematic phase was observed. Growing the cholesteric phase between parallel plates with $d \ll p_{00}$ has resulted in textures quite different from Fig. 1 and typically shown in Fig. 6.

It is difficult to reconcile the lack of variation in contrast when the sample is rotated above the polarizer with this model. If we assume that light scattered away from the χ disclination is depolarized, this

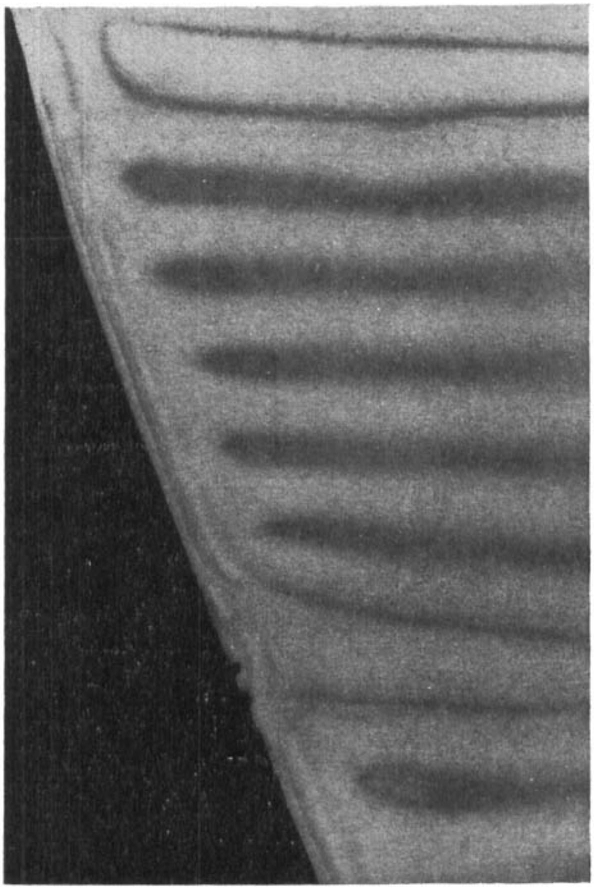


Figure 6. Typical texture observed when the cholesteric phase is formed from the isotropic state between glass plates whose thickness $d < p_{00}$. Here the thickness is 5μ, whereas $p_0 \sim 25\mu$. The texture was grown in vacuo.

may account partially for this effect, it does not, however, explain why the brightest contrast occurs below the surface of the sample. Consequently, a more likely reason is that the model is only partly correct since we have assumed a planar configuration, i.e. $n_x = 0$. We will show (in the next section) that in order to minimize the Frank Energy correctly, $n_x \neq 0$ near the surface $z = \pm d/2$ and $x = \pm p_0/4$.

3. Considerations on the " Molecular Field " Condition

The Euler Lagrange minimization equations of the Frank energy are, in the isotropic case:

$$K[\nabla^2\mathbf{n} - 2q_0 \operatorname{curl} \mathbf{n}] = \lambda \mathbf{n}, \tag{16}$$

where λ stands for a Lagrange multiplier relative to the condition $n^2 = 1$. De Gennes,⁽⁹⁾ who calls $\mathbf{h} = K[\nabla^2\mathbf{n} - 2q_0 \operatorname{curl} \mathbf{n}]$ the molecular field, in analogy with magnetism, has pointed out that a constrained solution like Eq. (3) does not necessarily satisfy Eq. (16).†

Using Eq. (16), the molecular field of the planar solution is

$$\mathbf{h} = \begin{cases} -2Kq_0 \sin\theta \dfrac{\partial \theta}{\partial z} \\ -K\left[\left(\dfrac{\partial \theta}{\partial x}\right)^2 + \left(\dfrac{\partial \theta}{\partial z}\right)^2 - 2q_0 \dfrac{\partial \theta}{\partial x}\right] \cos\theta \\ -K\left[\left(\dfrac{\partial \theta}{\partial x}\right)^2 + \left(\dfrac{\partial \theta}{\partial z}\right)^2 - 2q_0 \dfrac{\partial \theta}{\partial x}\right] \sin\theta. \end{cases} \tag{17}$$

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† It is clear from Eq. (16) that the molecular field is satisfied for a cholesteric in the case of any planar configuration of the molecules and then only if $\theta = \theta(x)$ only, where X is the twist axis. As soon as θ becomes a function of any other variable perpendicular to the twist axis (because for example the pitch $q_0(y,z)$) the planar solution becomes unstable. When we heat a cholesteric sample in the homogeneous texture (twist axis perpendicular to the glass plates with uniform twist q_0, as we approach within 1 or 2 degrees C of T_C, the striped texture appears. The appearance of this texture (axis parallel to the glass plates) can be understood in terms of the molecular field argument. Heating the sample results in a change in pitch which may not be uniform with respect to coordinates in the plane of the sample, consequently the molecular field is no longer directly parallel to **n** and the molecules experience a torque about an axis in the plane of the sample—eventually resulting in what we have termed a finger-print texture very similar to Fig. 1 but with the stripes twisted into confocal domains.

Clearly, $h_x \neq 0$. For the molecular field to be partly satisfied, we require

$$|h_x| < |h_y^2 + h_z^2|^{1/2}. \tag{18}$$

(That is continuing the magnetic analogy, we consider h_x as an applied field on a medium subjected to a field h_y, h_z under which it is in equilibrium).

Now,

$$\begin{aligned}\frac{\partial\theta}{\partial z} &= 2q_0 \sum_n (-)^n \frac{\sinh 2nq_0 z \sin 2nq_0 x}{\cosh nq_0 d} \\ &\cong \frac{-q_0 \sin 2q_0 x}{\cosh q_0(d-2z) + \cos 2q_0 x}\end{aligned} \tag{19}$$

providing $d \sim p_0$, $z \sim d$ but $z \neq d$ and $2q_0 x \neq n\pi$, $n = 0, 1, \cdots$.

Similarly,

$$\frac{\partial\theta}{\partial x} = q_0 \frac{\sinh q_0(d-2z)}{\cosh q_0(d-2z) + \cos 2q_0 x}. \tag{20}$$

Certainly if $z \sim 0$ and $d \sim p_0$, $\partial\theta/\partial z \cong 0$ and consequently $h_x = 0$ for any θ.

In Fig. 7, we plot the line along which

$$2q_0 \sin\theta \frac{\partial\theta}{\partial z} = \left[\left(\frac{\partial\theta}{\partial x}\right)^2 + \left(\frac{\partial\theta}{\partial z}\right)^2 - 2q_0\left(\frac{\partial\theta}{\partial x}\right)\right].$$

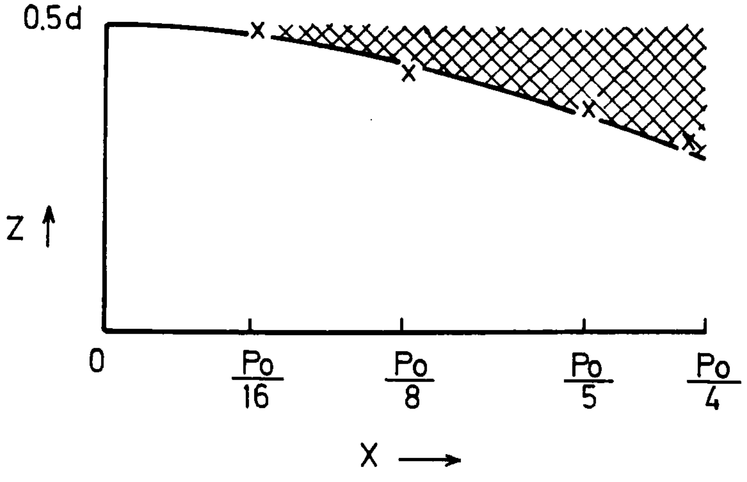

Figure 7. The dashed area is the region for which the x-component of the molecular field is larger than the y and z components. Here we expect that the director field will no longer be planar i.e. $n_x \neq 0$. The thickness $d \sim p_0$.

The planar solution as envisaged by Eq. (3) clearly cannot be stable in the cross-hatched area where $h_x > \surd \mid h_y{}^2 + h_z{}^2$.

In Fig. 8, we show a possible solution to our problem in which the χ of the naive model is replaced by a pair of disclinations called λ and $\tau^{(2)}$ (see Appendix C). The minimum distance between such a pair of disclinations $= p_0/4$. By comparison with Fig. 7, we see that near $x = p_0/4$, the distance along z for which the torque of the molecular field on the director is non-negligible $\sim p_0/4$.

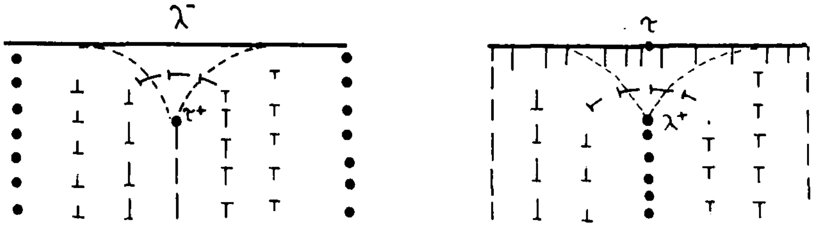

Figure 8. Repartition of the director **n** in the vicinity of a pair (*a*)λ^-, τ^+ and λ^+, τ^-. The smaller dashes indicate the region in which the molecular field is not satisfied (Fig. 7).

Another example of a splitting of a χ, not connected with the geometry studied here but interesting because it may be related to a molecular field effect, is provided by considering a singularity along the cholesteric axis. Details are given in Appendix B.

4. Conclusion

There are still many problems to be resolved concerning the cholesteric domain texture. In particular we mention (a) we have yet no clues as to why this texture should grow so that the twist axis is parallel to the isotropic boundary and (b) the role that the solvent plays in controlling the optical contrast. However, the results of our calculation seem to indicate that in a configuration such as shown in Fig. 9 (taken in monochromatic light), it is likely that the bright lines are caused by the presence of the τ^+ disclination located $\sim \frac{1}{4}p_0$ below the surface and which we have found necessary to introduce from molecular field considerations (Eq. 18). At the surface we noticed no discontinuity, but a λ^- is supposed to exist. These are disclinations in the plane of the sample.

Figure 9. Large pitch cholesteric ($\sim 25\ \mu$) held between rubbed glass plates ($d \sim 25\ \mu$). Focus 5 μ below the surface of the sample, viewed between crossed polaroids. The points where three bright lines join defines a λ^- disclination viewed head on. Where a bright line ends we have a λ^+, again with axis perpendicular to the plane of the sample. The bright line is caused by scattering and depolarization of light by the τ^+ disclination located $\sim p_0/4$ below the surface running parallel to the glass plates. No discontinuity is observed at the surface.

In the body of the sample, the cholesteric twists as suggested by Eq. (3). It is feasible then that the two types of disclinations visible in Fig. 9 perpendicular to the sample, and which appear as functions of the stripes are the λ^+ and λ^- variety (Figs. 13(b) and 12(d)). It is interesting to note that according to contrast calculations by Taupin,(8) this is the only way to observe a λ, i.e. outlined by the presence of the τ at the surface. The problem of the proposed fitting of the vertical λ's with the horizontal pair is yet to be investigated.

The configuration we propose (Fig. 8) suggests that $d > p_0/2$ at least.

Acknowledgements

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Appendix A

Variation of pitch with concentration for a Nematic Cholesteric Mixture.

Let $K_{22}(N)$, $K_{22}(C)$ be the elastic constants of twist for the nematic and the cholesteric component respectively. Then let us assume that the free energy density is given by

$$F = (1-C)\left(\frac{\mathrm{d}\theta}{\mathrm{d}z}\right)^2 K_{22}(N) + C\left(-\frac{\mathrm{d}\theta}{\mathrm{d}z}+q_0\right)^2 K_{22}(C) + F_0 \qquad \text{(A1)}$$

where F_0 represents terms independent of the pitch ; C is the volume fraction of cholesteric, Z is the twist axis. So, we put $\mathrm{d}\theta/\mathrm{d}z = \pi/p$ and find the value p which minimizes F, i.e.

$$\frac{\partial F}{\partial p} = 0, \qquad p = [K_{22}(N) - C[K_{22}(N) - K_{22}(C)]]\,\frac{p_0}{CK_{22}(C)} \qquad \text{(A2)}$$

where $p_0 = \pi/q_0$ is the natural half pitch of the pure cholesteric ~ 2000 Å if $K_{22}(N) = K_{22}(C)$, then $p = p_0/C$ i.e. the pitch is linear in $1/C$ which is observed.(10) If

$$K_{22}(C) \ll K_{22}(N), \qquad p = \frac{(1-C)}{C}\,\frac{K_{22}(N)}{K_{22}(C)}\,p_0.$$

Note that the $K_{22}(x)$ can depend on concentration too. One can apply this analysis to two cholesterics each with natural pitch q_1 and q_0 respectively. In the simple case where $K_{22}(C_1) = K_{22}(C_2)$

$$\frac{\pi}{p} = (1-C)q_1 + Cq_0$$

if $q_1 = -q_0$, $\pi/p = 0$ when $C = 50\%$ (racemique), if not, net optical rotatory power p is given by $p = \pi/((1-C)q_1 + Cq_0)$ as is observed.(10)

However, in the case where the optically active compound is not cholesteric (e.g. Canada Balsam added to MBBA has been observed(6) to give exactly the same sorts of textures as a cholesteric would even though it is not cholesteric), this analysis does not hold. It would be interesting to know if the pitch concentration relation is similar. When $p = p_0/C$ it should be borne in mind that $p_0(T)$, T = temperature. For example 4% cholesteryl benzoate added to PAA results in a $p \sim 50\,\mu$ whereas 0.4% of cholesterol propionate added to MBBA gives a very small twist ~ 6–8 μ (see Fig. 10).

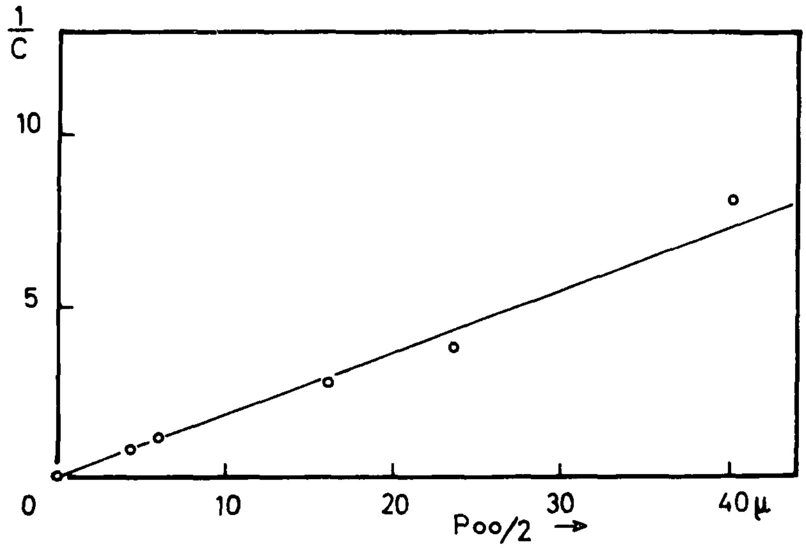

Figure 10. (Concentration)$^{-1}$ as a function of pitch, $p_{00}/2$, measured in the Cano Wedge.

Appendix B

If **n** is constrained to stay perpendicular to the cholesteric axis, Φ being the angle of **n** with a constant direction, such a χ singularity along the cholesteric axis z is described by the equation

$$\Phi = S\theta + q_{00}z \qquad \text{(B1)}$$

The configuration is the same as the configuration proposed by Frank for a singularity in a nematic, but twists along the cholesteric axis. It is easy to see that it leads to a molecular field

$$\mathbf{h} = (0, 0, h_z), \qquad h_z = -2Kq_0\frac{S}{\rho}\sin(S-1)\theta + q_{00}z) \qquad \text{(B2)}$$

which becomes infinite on the axis of the singularity. The region in which h_z is large enough to rotate n towards the axis is of the order of q_0^{-1}. More precisely, we can get an idea of the configuration near the axis by solving Eq. (16). In spherical polar coordinates, $n_\rho = \sin\phi\sin\psi$, $n_\theta = \cos\phi\sin\psi$, $n_z = \cos\psi$, we have

$$\sin\psi\nabla^2(\phi-\theta) + 2\cos\psi\nabla\psi\cdot\nabla(\phi-\theta) + 2q_{00}\mathbf{n}\cdot\nabla\psi = 0$$
$$\nabla^2\psi - \sin\psi\cos\psi(\nabla\phi)^2 - 2q_{00}\sin\psi\mathbf{n}\cdot\nabla(\phi-\theta) = 0 \qquad \text{(B3)}$$

We study successively the solutions near the axis (ψ small) and far from the axis ($\omega = \pi/2 - \psi$ small). We suppose the pitch to be large, so that we can insert the " unperturbed " values of ϕ and ψ in Eq. (B3) in the last term.

(a) ψ small we get

$$\psi_z{}' = 0, \qquad \psi_\theta{}' = 0,$$

$$\rho^2\psi''_{\rho^2} + \rho\psi_\rho{}' - \psi[(S-1)^2 - q_{00}^2\rho^2] = 0. \tag{B4}$$

A non singular solution near the axis is

$$\psi \propto J_{S-1}(\xi)$$

where $$\xi^2 = \rho^2 q_{00}^2.$$

$J_{S-1}(\xi)$ is the Bessel function of order $S-1$ and oscillates with a periodicity of the order of p_{00}.

(b) ω small we get

$$\omega(\rho, z, \theta) = \omega(\rho)\sin((S-1)\theta + q_{00}z)$$

$$\rho^2\omega''_{\rho^2} + \rho\omega_\rho{}' - 2\rho^2 q_{00}^2\omega = 2q_{00}S_\rho. \tag{B6}$$

A general solution is

$$\omega = aI_0(\xi) + b\kappa_0(\xi) + iS\frac{\pi}{\surd 2}\,\mathrm{sgn}\,(q_{00})\mathscr{H}_0(-i\xi) \tag{B7}$$

where $\xi = \rho\,|\,q_{00}\,|\,\surd 2$, I_0 and κ_0 are modified Bessel functions and $_0(\xi)$ the Struve function of zero order.

The solution which tends to zero for ξ infinite is

$$\omega = \frac{S\pi}{\surd 2}\,\mathrm{sgn}\,(q_{00})[-I_0(\xi) + i\mathscr{H}_0(-i\xi)] \tag{B8}$$

and behaves at infinity like the quantity

$$\omega_\infty(\xi) = -S\surd 2\,\mathrm{sgn}\,(q_{00})\left(\frac{1}{\xi} + \frac{1}{\xi^3} + \frac{3^2}{\xi^5} + \frac{3^2\cdot 5^2}{\xi^7}\cdots\right) \tag{B9}$$

If we look at a pattern of the configuration of the molecules in a plane θ = constant, we note that the solution has a periodicity $p_0/2$ along the cholesteric axis, each period having an internal element of symmetry (See Fig. 11), and that the pattern rotates helically along the axis with a pitch $p = p_0(1-S)$. It is evident (Fig. 11) that passing from the configuration for ξ infinite towards the configuration, essentially nematic, on the axis, requires the introduction of singularities, which are of the λ and τ types. A similar problem has already been considered in Ref. (2) under the heading: paires hélicoïdes proches de l'axe, and we see that our calculation leads to a result similar to that drawn in Fig. 12(d) Ref. (2).

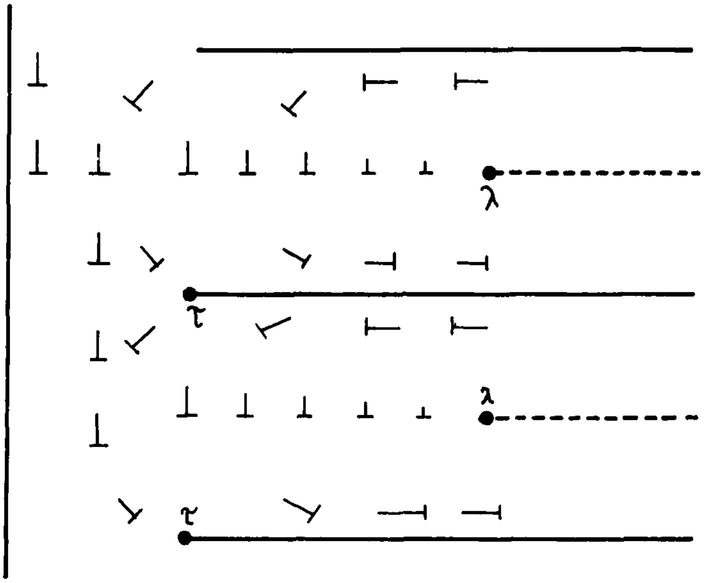

Figure 11. Section pattern of the dissociation of a χ located along the cholesteric axis.

Appendix C

In this section, we wish to recall the topological features of the simplest types of straight disclinations λ, τ and $\chi^{(2)}$ which we have referred to in the preceding text.

We define the disclination line L as being the limit of a cut made into a cholesteric. We assume in this process that the molecules are not disturbed by the cut. To effect this, we postulate the existence of suitable torques at the two surfaces S_1 and S_2 created by the cut, S. These torques keep the molecules firmly anchored to S_1 and S_2. We then displace S_1 and S_2 (see Fig. 12(a) and (b)) by rotating S_1 by $+\pi/2$ (counter-clockwise) and S_2 by $-\pi/2$ (clockwise). The net effect is a rotation of π which corresponds to a symmetry rotation for cholesterics. The surface formed by S_1 and S_2 is now clad with

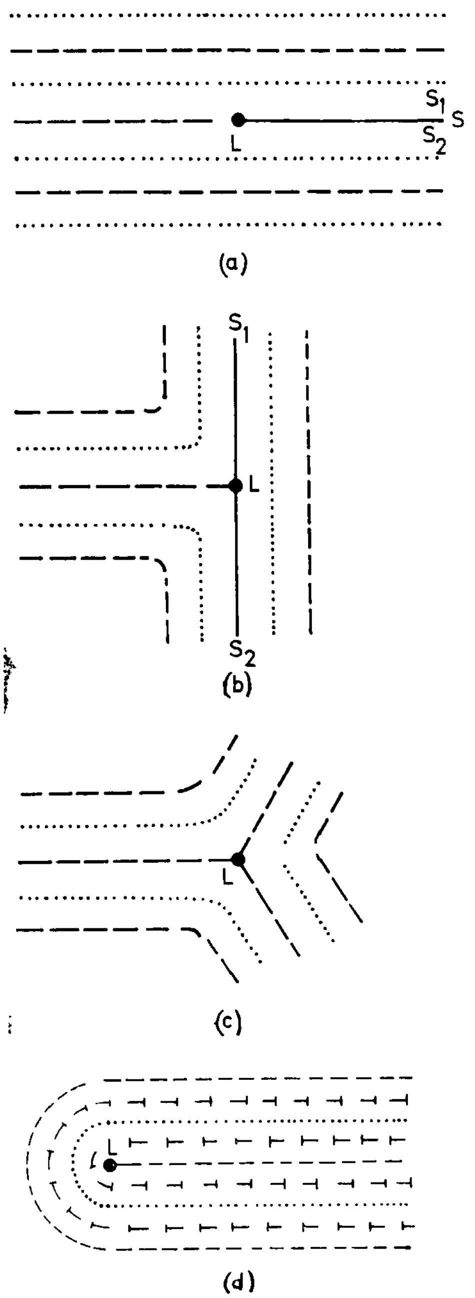

Figure 12. The Volterra process for a τ disclination. The configuration for τ^+ is shown in 12(c) and τ^- in 12(d).

perfect cholesteric (Fig. 12(b)) and the whole system allowed to relax viscuously (Fig. 12(c)). If the line L lies in a cholesteric plane (as shown in Fig. 12), two simple cases can be considered. In the first case, the molecules in the cut plane are perpendicular to L. This case has been termed a τ^- (Fig. 12(c)) where τ denotes the transverse orientation of the molecules and the minus sign indicates that we have added material to our originally perfect cholesteric to arrive at our final configuration. In the second simple case, the molecules on the cut plane are parallel to L. This has been called a $\lambda^- - \lambda$ for longitudinal (Fig. 12(d)).

To arrive at disclinations of positive sign, we rotate S_1 by $-\pi/2$ and S_2 by $+\pi/2$, " glue " along the line of the cut S and then remove the excess " flaps ". Disclinations of positive sign result. Again, considering the two simple cases for a line which lies in a cholesteric

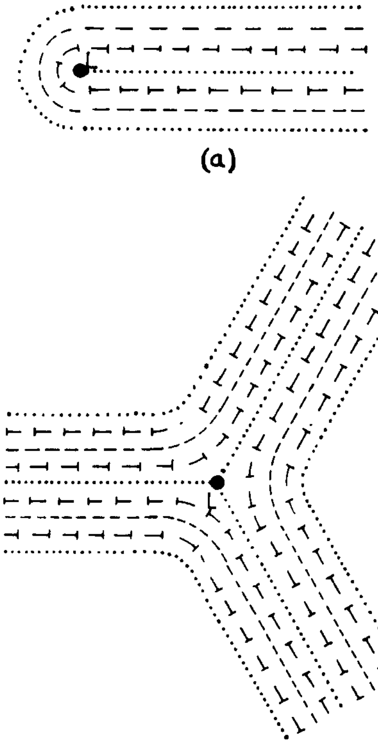

Figure 13. The configurations for a λ^+(13(a)) and λ^-(13(b)).

plane, we term a line a τ^+ (Fig. 13(a)) when the cut S takes place in a plane in which the molecules are perpendicular to the line L and a λ^+ (Fig. 13(b)), when parallel to L.

When the line L is parallel to the cholesteric axis, we term it a χ. In this case we expect the same sorts of disclinations as for a nematic. For each cholesteric plane,(1) $\psi = S\theta + \psi_0$, where ψ is the inclination of the molecules as the azimuthal angle θ is swept out. S is the strength of the disclination, $S = \pm\frac{1}{2}, +1, \ldots$ and ψ_0 is given by $q_0(z)$(2) where $q_0 = 2\pi/p_0$, p_0, the pitch and z the co-ordinate of the plane along the twist axis.

A χ may assume any shape topologically but a single λ or τ must be straight. The possibility does exist, however, that if λ's and τ's of opposite sign are coupled, i.e. a λ^+ and λ^- or λ^+ and τ^-, these pairs may then take any shape. See Ref. (2) for a more complete description of disclination lines in a cholesteric.

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