Waves and Symmetry
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Defects in Liquid Crystals

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By way of introduction

In the very year that C. V. Raman was born, an important discovery was made which called for a revision of long-held ideas on the melting of crystals. It was observed that crystals of certain organic compounds did not melt directly into the liquid, but went through an intermediate state[1]

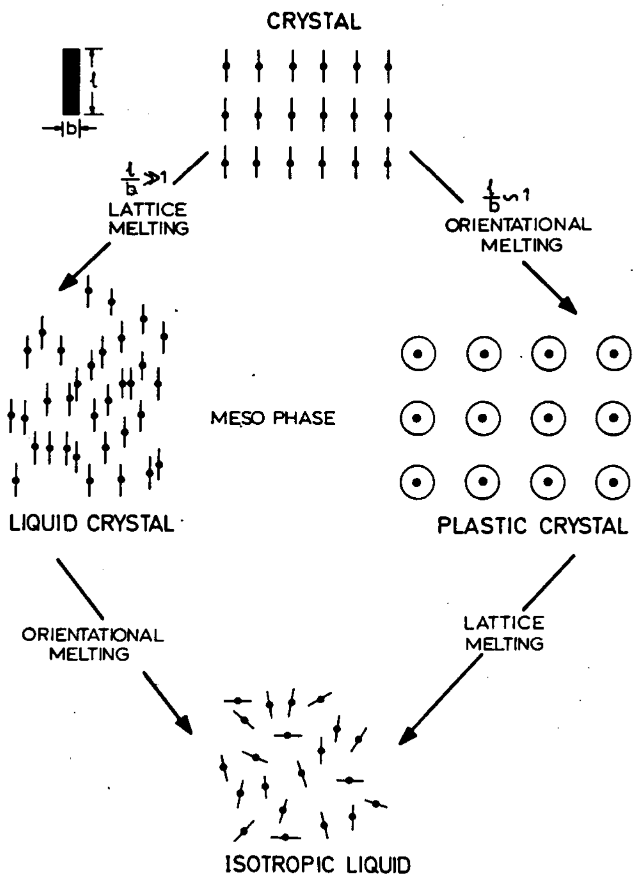

Figure 1. A schematic representation of the melting phenomena in mesophases.

(for early history, see Kelkar and Hatz[2]). Substances exhibiting this strange melting behaviour were invariably made up of very anisotropic rod-like molecules. In figure 1 is shown a simple way of understanding the essence of this phenomenon. To start with, we have a crystal made up of rod-like molecules. This crystal first melts into a state in which the lattice structure, i.e., the positional order, has disappeared altogether but the molecular orientations are still preserved. On further heating even this orientational order disappears. This intermediate state has an axis of cylindrical symmetry with an orthogonal mirror. It is unlike the classical liquid which is spherically symmetric, and moreover it can flow like a liquid as it lacks lattice order. In view of this combination of crystal-like anisotropy and liquid-like flow these phases were termed as liquid crystals.

Mesophases may also occur even when the molecules are not highly anisotropic, but more or less spherical. This is also shown in figure 1. Here the orientational order breaks down first, leaving the lattice order intact. On further heating the lattice order also disappears. Such mesophases are called plastic crystals.

The liquid crystal structure shown in this figure is the simplest of the liquid crystalline phases. It is called the nematic liquid crystal. The preferred direction of alignment of the molecules is referred to as the director. The director can be made to vary slowly and smoothly from place to place. Of course, this distortion calls for elastic energy.

Topological defects

Disclination Lines

We now have enough ingredients to construct topological defects in nematics. The necessary procedure to get defects in any given system was worked out long back by the Italian mathematician Volterra. In the present case we have only rotational symmetries and this results in disclinations

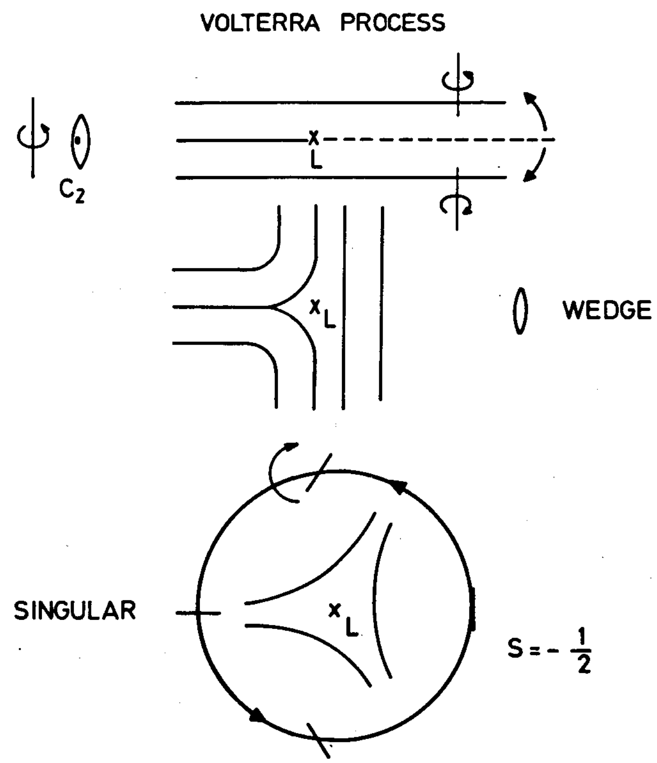

Figure 2. The Volterra process for creating a $S = -\,^1\!/_2$ wedge disclination in nematics.

only. Figure 2 gives the main steps involved in the Volterra process[3,4]. We imagine the undistorted nematic to be cut by a semi-infinite plane ending in a line L which is perpendicular to the director. Then the Volterra process demands that we rotate molecules on one face of the plane of cut, relative to the molecules on the other through a rotational symmetry element of the nematic. Rotation of the molecules about the director, i.e., the cylindrically symmetric direction, will leave the system unaltered. Let us see what we get by employing the orthogonal 2-fold symmetry element. In particular we can rotate the molecules about the 2-fold parallel to the line L by bending the director on either side of the cut respectively through $+\pi/2$ and $-\pi/2$. This creates a wedge with no material whatever in the other half of the space. The next step in the Volterra process is to fill up this space with an undistorted nematic so placed that the directors match smoothly everywhere excepting at the centre. Later we allow the system to relax. Figure 2 shows a section perpendicular to L of this final state. This object has some beautiful properties.

(i) If we go round the line L in a certain sense we find the director also to rotate along the path but in the opposite sense and on the completion of the circuit it would have rotated through π. This unique property is topological in origin. The ratio of the rotation undergone by the director to the rotation we cover during the circuit is equal to $-\pi/2\pi = -1/2$. This ratio is called the strength 'S' of the defect. The defect itself is termed a $-1/2$ wedge disclination. If on the other hand we had rotated the two faces respectively through $-\pi/2$ and $+\pi/2$ then

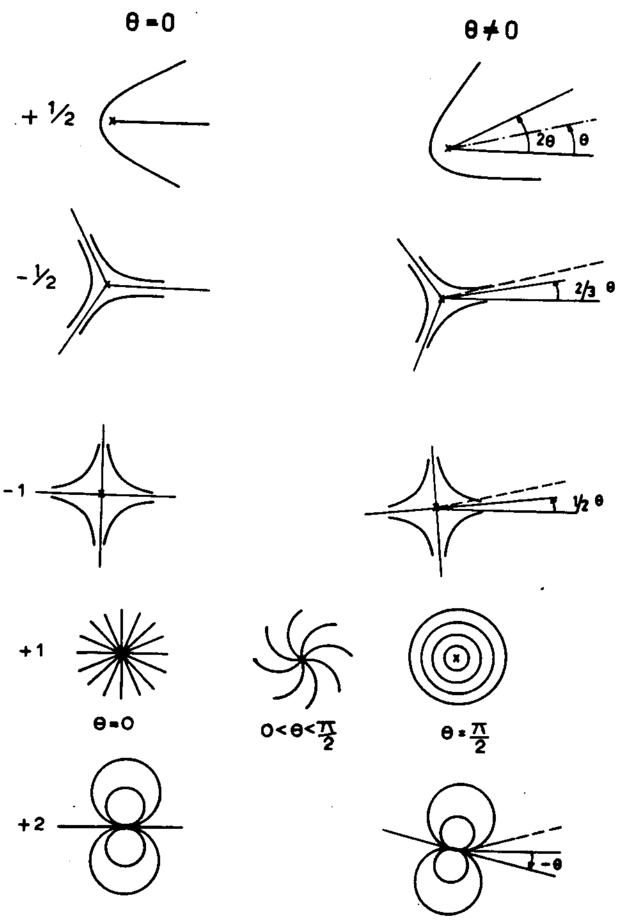

Figure 3. On the left is shown wedge disclinations together with their strengths. On the right is shown the effect of a rotation through θ about the disclination line.

instead of a gap we would have got overlapping regions. Removal of overlap results in $S = +1/2$ wedge disclination.

(ii) If we reach the centre of this pattern from different directions we end up with different director orientations, implying a singularity on the line L.

(iii) The structure has elastic energy arising from director distortions.

If we had rotated about the 2-fold which is perpendicular to L and the plane of cut, then we would not have introduced any wedge or overlap but a twist in the material. Such defects for obvious reasons are called as twist disclinations.

It is easy to see that a $\pm N\pi$ rotation (N being an integer) between the two faces of the cut gives defect of strength $\pm N/2$. Figure 3 shows some of the wedge disclinations so created. This figure also depicts the effect of imposing a rotation about the axis L. Wedge disclinations of strength less than $+1$ undergo a body rotation by an amount that differs from defect to defect. Interestingly $S = +1$ defect undergoes structural modifications, changing from all radial to all circular with intermediate equiangular spirals, as the imposed rotation changes from 0 to $\pi/2$. However, defects of higher strength also experience a body rotation but in the opposite sense.

Effect of rotation about a direction perpendicular to L is shown in figure 4. Under a rotation through $\pi/2$ a wedge disclination gets transformed to a twist disclination of the same strength. On a further rotation through $\pi/2$ it becomes again a wedge disclination but of opposite strength, i.e., an anti-defect. This operation reveals the important topological equivalence, not only between a wedge and a twist disclination but also between a defect and an anti-defect.

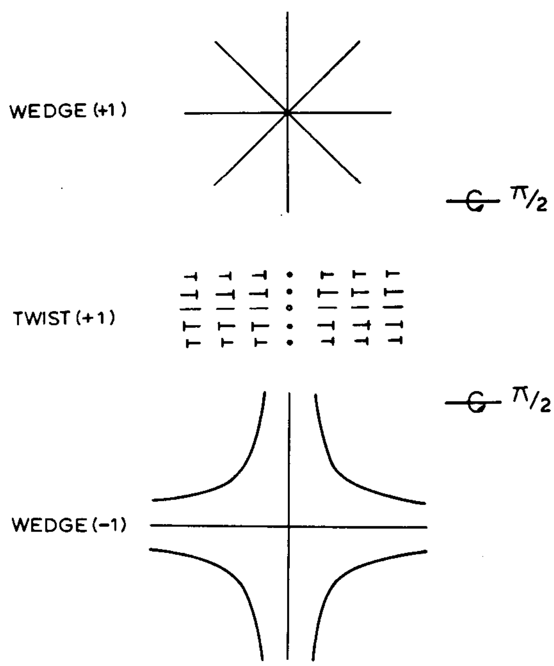

Figure 4. Conversion of a $S = +1$ wedge disclination into a twist disclination of same strength by a $\pi/2$ rotation about an axis perpendicular to the line L. A further rotation of $\pi/2$ about the same axis converts the twist disclination into $S = -1$ wedge disclination.

It should be noted that none of the geometrical operations considered so far can remove the singularity on L. It therefore appeared spectacular when a geometrical transformation, that could remove the singularity, was discovered[5,6] in the early 70's. In figure 5 we show the salient aspects of this important work. We take the $S = +1$ all radial defect. Now relax the restraint that the director be confined to a plane (which in this case is perpendicular to L). Allow the director to

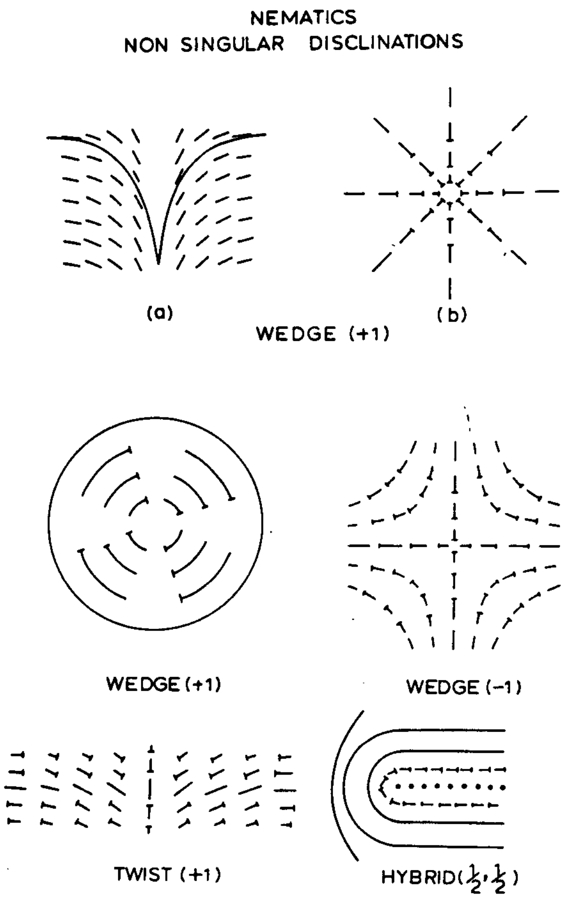

Figure 5. Non-singular disclinations in nematics.

smoothly go over to direction of L as we approach the centre, thus ending up in a structure that is strictly non-singular. Subjecting this object to a rotation $\pi/2$ about L results in a $S = +1$ all circular non-singular configuration. Rotation about an axis perpendicular to L through $\pi/2$ gives a non-singular $S = 1$ twist disclination. A further rotation through $\pi/2$ about the same axis yields a non-singular $S = -1$ defect. Thus a line defect of any type (wedge or twist) and of any sign but of unit strength is always non-singular. This result can be generalized to mean that any integral line defect is non-singular. This, however, does not mean that we should have only twist or wedge defects. In fact we can even have a hybrid of the two types, each of strength 1/2 which is again non-singular as shown in the same figure. But we have no such possibility of eliminating the singularity in the case of half integral defects. And they are line singularities.

Disclination Points

At this stage we recall the cases of crystal dislocations and fluid vortices, which are the other line singularities that we are familar with. It is almost text book information that these line singularities either end at the surfaces of the material or on themselves. The very same properties are also true for our line singularities. Let us see what we get when they end upon themselves forming loops. In figure 6 we have shown this explicitly for a $S = +1/2$ loop. We can easily visualize this loop to shrink continuously and collapse into a spatially radial hedgehog-like structure. Here we find the

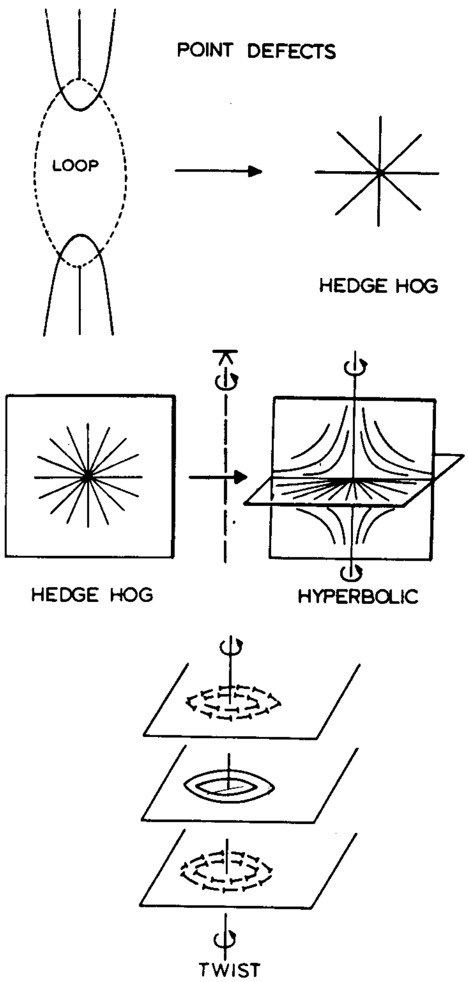

Figure 6. Generation of a hedgehog point defect and its conversion to a hyperbolic and twist point defects.

singularity to reside at the centre of the pattern. Thus we get a point singularity by allowing a singular disclination loop to shrink[4]. A rotation of π about an axis through its centre transforms a hedgehog to a hyperbolic point defect. However, a rotation of $\pi/2$ results in what might be called a twist point defect.

Experimental Facts

All these exercises in geometry are not futile. In point of fact we show in plate 1 what in the liquid crystal jargon is called as a Schlieren texture. This pattern is obtained when a nematic sandwiched between two plates is viewed under a polarising microscope. One can work out the director pattern from this optical information. We find any two-brush point to be a defect of strength $\pm\, ^1\!/_2$, whereas a four-brush point has a strength of $\pm$ 1. Careful experiments also show that at the centre of the four-brush structure the birefringence continuously decreases implying a tilt of the director out of the plane. Also experimentally the $S = 1/2$ singular lines reveal themselves optically as threads or nematods (in Greek) when seen in a perpendicular direction. That is how these phases came to be described as nematics. It must be mentioned in passing that even the three types of point singularities discussed earlier are also seen in the laboratory. Thus experiments do confirm the important conclusions of our analysis.

Poincaré Structures

That a singular line should either end at surfaces or on itself has exceptions[7]. Nabarro undertook the task of working out defects in nematics, by a technique developed long back by Poincaré while analysing possible defect states in the velocity fields of fluids. In addition to getting all the above defects Nabarro found that structures of the type shown in figure 7 are also allowed. The first two structures have a cylindrical symmetry with $S = \pm 1/2$ director pattern in the meridional plane. We can even have $+1/2$ structure in one plane and $-1/2$ in the orthogonal plane. Poincaré structures are truly unique. Firstly they are singular for $Z < 0$ and are strictly non-singular for $Z > 0$, i.e., a singular line ends in the body of the material. Secondly the line singularity has a strength of ± 1.

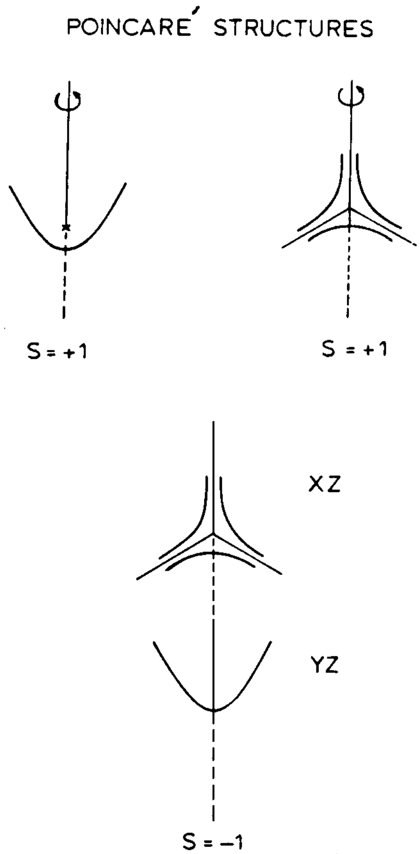

Figure 7. Poincaré defects of different strengths.

A method of generating and studying these Poincaré defects is illustrated in figure 8. We consider a homeotropically anchored (i.e., director perpendicular to the plates) nematic with negative diamagnetic anisotropy, in a magnetic field applied parallel to the director. The field tries to pull the director away from the imposed alignment, but the elastic responses oppose any such distortion. At low fields elasticity wins and the state is undistorted. But above a threshold, the field wins over elasticity and we get the first configuration. At the centre of this cylindrically symmetric non-singular distortion the director still opposes the field. At higher fields this region also breaks down into what is shown in the next diagram. A singular line of strength of $+1$ terminates in the body of the material at two unlike Poincaré structures.

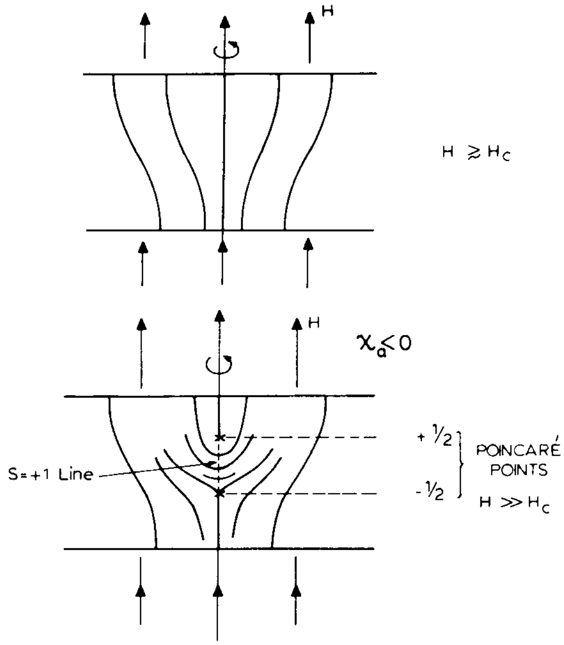

Figure 8. Generation of Poincaré defects.

Solitons

We may wonder what might happen when the material has positive diamagnetic anisotropy. For the field to be effective it should act perpendicular to the director. Here also, above a threshold the director tilts, in the plane of the field and the initial orientation. Since this tilt can be positive or negative we have the possibility of their simultaneous existence. Two such degenerate solutions get connected by a non-singular wall. When the plates are moved to infinity this wall goes over to the Helfrich 'splay' wall[8] with the director turning through π inside the wall, which has a finite field-dependent thickness. Even 'Bend' and 'Twist' walls are possible. Such walls are termed as planar solitons[9].

Effects of Lattice Symmetry: Smectics

It was pointed out that nematics are the simplest of the liquid crystals. Next in the order of complexity is a smectic liquid crystal. Referring back to figure 1 we see that we got a nematic by melting the three-dimensional lattice completely. However, if lattice melts in the XY plane but not in the Z direction, then we end up with a nematic-like orientational order with a superimposed lattice order along the director (see figure 9). We have a fluid-like positional order in the perpendicular direction. This structure is called a smectic liquid crystal. The smectic shown in figure 9, referred to as smectic A, is the simplest of a large class of smectics that are known to exist. Such structures exist in lyotropics (smectic is a Greek word for soap, which is a multicomponent solute-solvent systems that are technically termed as lyotropics) as well as thermotropics.

Like a classical nematic, smectic A has a cylindrical rotational invariance along the director with an orthogonal 2-fold axis. But the position of this 2-fold axis is confined to either the centre of any smectic layer or exactly between any two smectic layers. In figure 9 we show the half line disclinations obtained as in nematics[3]. Interestingly here we have two different types of positive or negative disclinations depending upon the position of the 2-fold axis. They are topologically different objects. Unfortunately, we cannot see these half disclinations optically. What we see experimentally is a disclination of strength $S = +1$. Let us look at this in detail. We construct here also the nematic equivalent of the all radial $S = +1$ disclination (see figure 9). If has an interesting feature. It is really singular. If we redo as in nematics the geometrical transformation of allowing the director to

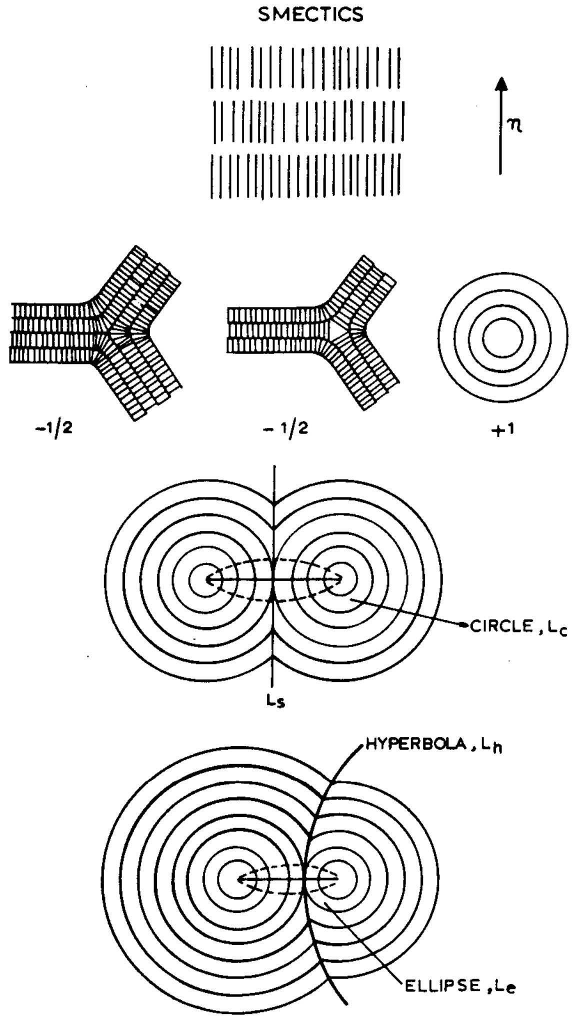

Figure 9. Disclination lines and loops in smectic A liquid crystals.

escape as it approaches the disclination line we will be introducing very large layer distortions. As this costs a lot of energy the system would rather live with the local singularity than accept globally intolerable layer distortions.

As in nematics, even here we may consider disclination loops. In nematics a loop like this would continuously shrink to yield a singular point. Here as the lattice structure prevents any such collapse, we get a new result. If the loop is circular (L_c), then a proper matching of toroidal smectic layers results in a straight line singularity (L_s) running through the centre of the loop and perpendicular to its plane. At every point on this line the smectic planes are conically tapered. We can also have a distorted version of this structure with the circular loop replaced by an ellipse (L_e), and the straight line by a hyperbola (L_h). These two conics are in orthogonal planes going through each others' focus[10]. This second solution has a beautiful topological property. Long back W. H. Bragg[11] showed that the whole of space can be filled with objects like this. Just as in nematics, these line singularities reveal themselves optically and we refer to such pattern of ellipses and hyperbolae as a focal conic texture. Of course depending upon how we look at it we see either ellipses or hyperbolae only as they are in orthogonal planes. The plate 2 shows one such view.

All these defects can be expected in any system that geometrically simulates a smectic A structure, i.e., a stacking of easily deformable layers. This fact is indeed supported by experimental facts.

Defects in systems of lower symmetry

Biaxial Nematics

(i) *Disclinations:* It was realised long back that nematic phases of even biaxial symmetry could exist. This prompted topologists to examine defects in such structures[12]. The simplest of the biaxial phases has an orthorhombic symmetry, i.e., three mutually perpendicular 2-fold axes.

The familiar Volterra process can be applied about any of the three 2-fold axes a, b and c. We may be tempted to conclude from this that for every disclination in the uniaxial nematic there are three distinctly different ones in biaxial nematics i.e., one each in $a - b$, $b - c$ and $c - a$ directors. This is true only for half integral disclinations. Let us see what we get for integral defects. In figure 10 we have depicted a $S = + 1$ defect in the $a - c$ director field. Just as in classical nematics let us try to eliminate the singularity by allowing the c director to tilt out of the plane into an orthogonal orientation. This process transforms this defect to a $S = + 1$ defect in $a - b$. In other words $S = + 1$

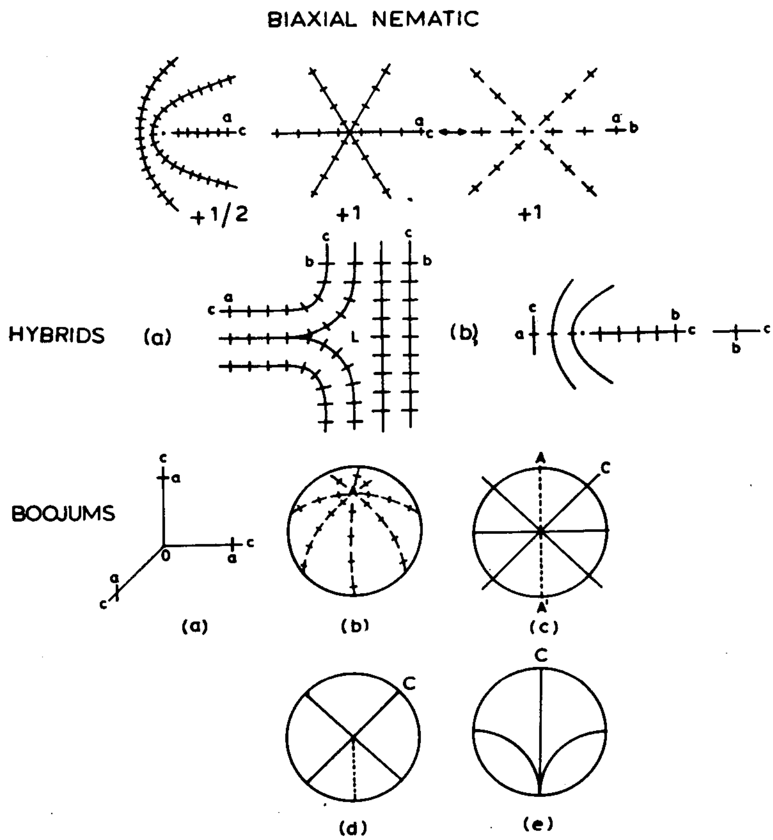

Figure 10. Defects in biaxial nematics: (1) Wedge disclination of strength $S = + 1/2$ and $S = +1$. (2) Volterra process for a hybrid defect together into a hybrid (+ 1/2, + 1/2). (3) Process leading to the formation of Boojums.

Plate 1. Schlieren texture in a nematic.

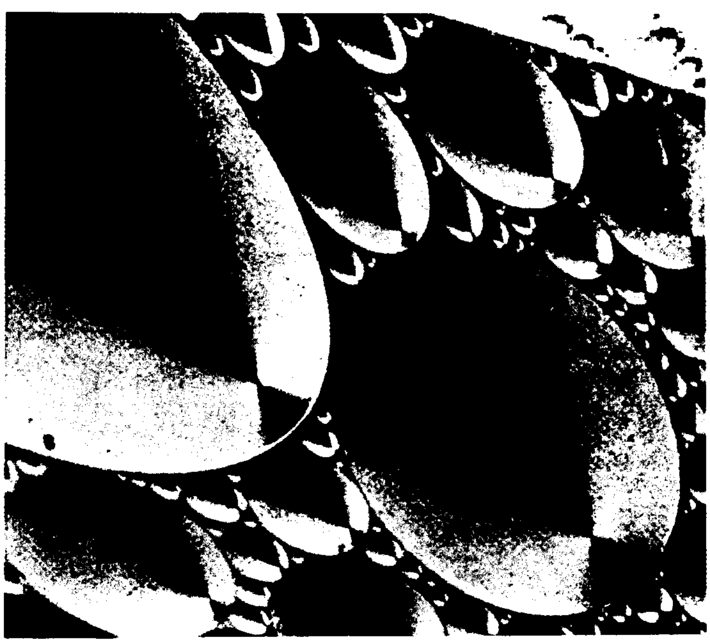

Plate 2. Focal-conic texture in a smectic A.

continues to be singular. Also the seemingly different $a - b$, $b - c$ and $c - a$ defects can be transformed to one another. Hence we have three distinctly topologically different types of half defects but only one type of $S = +1$ defect. Even here a wedge defect goes into a twist defect or a wedge anti-defect under a rotation through $\pm \pi/2$ or $\pm \pi$ about an axis perpendicular to the disclination line.

(ii) *Hybrids* : The biaxial symmetry also implies another type of defect[13,14]. The essential step involved in the construction of this new defect is also shown in figure 10. We open out a wedge about one of the three 2-fold axes, say the b-axis. As we have 2-fold symmetry about a, b or c axis, the c director on the two arms of the wedge can be rotated further through $+\pi/2$ and $-\pi/2$ respectively (i.e., a relative twist of π about c-axis) resulting in the $c - b$ orientation along the arms. We now juxtapose on the empty half space the biaxial nematic with the orientation $b - c$. After this step, we allow the system to relax. We first rotated about L and then about an orthogonal direction. Thus this defect can also be looked upon as a hybrid disclination having a twist and a wedge component each of strength half. We show a (+ 1/2, + 1/2) hybrid in the figure. We can construct different hybrids by selecting different strengths for the wedge and twist components. We can even construct a twist-twist hybrid.

The fact that $S = \pm 1/2$ and $S = \pm 1$ disclinations are singular may force us to conclude that in general both integral and half integral defects are singular. The beauty with biaxial nematics is that such generalisations are invalid. In figure 11 we show how a $S = +2$ defect in $a - b$ can be deformed to remove the singularity. The c axis smoothly turns in the meridional plane through π as we reach the disclination line. In this process we end with the same orientation at the centre irrespective of the direction of approach to L. Therefore the conclusion to be drawn is that half integral and odd integral are singular while even integrals are non- singular. Also a hybrid with the total of

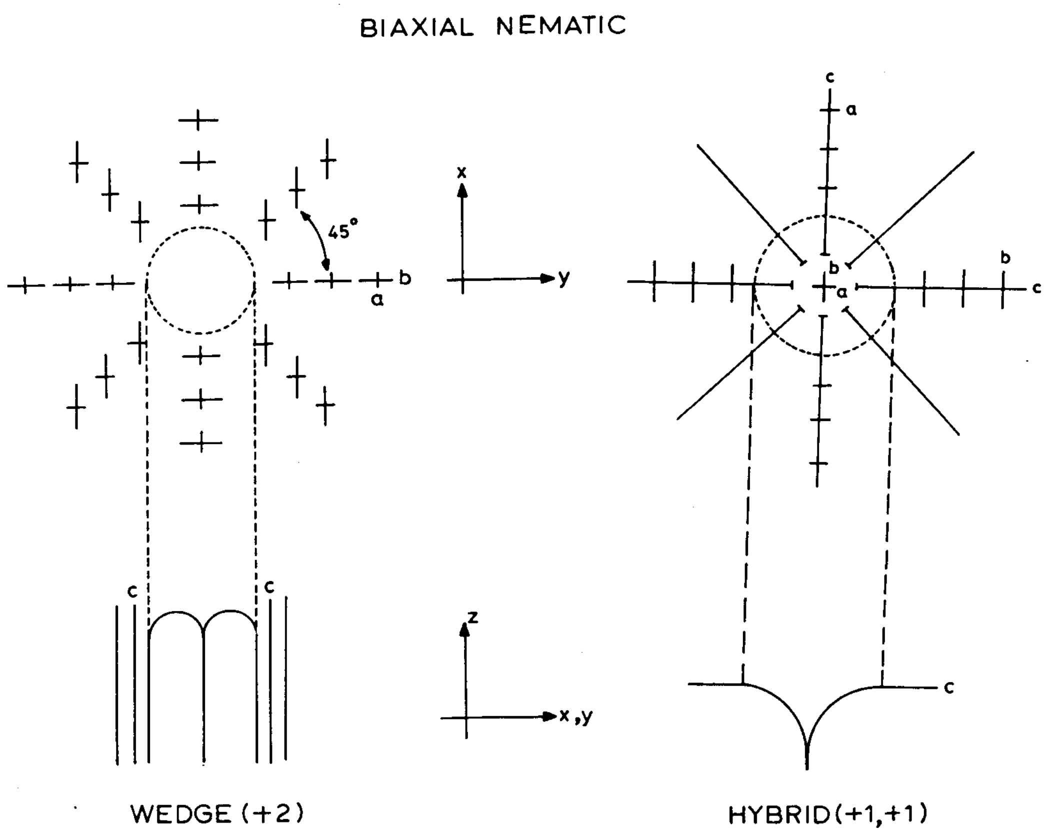

Figure 11. The c director escape in a disclination of strength $S = +2$ and a hybrid (+1, +1) resulting in non-singular structures in biaxial nematics.

strength of both the components adding upto an even integral, is also non-singular. The same figure depicts this for a hybrid whose twist and wedge components have the same strength $S = +1$.

(iii) *Monopoles and Booja* : As in classical nematics we allow a $S = +1/2$ loop in $a - c$ to shrink to a point (figure 10) to get the c director in the radial hedgehog configuration. But at every point the directors a and b get mapped on to the surface of a sphere. In any such mapping we end up with two poles each of configuration $S = +1$. Of course the two poles occur on every sphere that can be drawn about the origin. Hence we conclude that from the centre of the hedgehog pattern in c, two singular lines in $a - b$ each of strength $+1$ emanate. We have a point defect in c connected to a pair of strings in $a - b$. We can topologically combine the two strings to one of strength $S = +2$ (this is also shown in figure 10) running from the centre to the surface. This is geometrically close to a Dirac monopole in structure, which is a point singularity in the magnetic field associated with a string of strength $S = +2$ in the vector potential. For this reason even here it is termed as a Dirac monopole.

A very similar defect is found in the case of superfluid He^3. And therefore even here as in He^3 one can go a step further and push the point singularity at the origin to the surface[15], thus eliminating altogether the line singularity. Such a structure [also shown in figure 10] is called a Boojum.

These beautiful theoretical results preceded the experimental discovery of the biaxial nematic phase. This phase was reported first in a three-component lyotropic system[16], and recently in thermotropic single component systems (Chandrasekhar *et al.*[17,18] and Malthete *et al.*[19,20] also reported a system in which they have claimed biaxiality).

Columnar Discotic Systems

Columnar discotic phases have a more complex structure than smectic A. In this case, we have a two-dimensional lattice with a fluid like structure in the third dimension in contrast to smectic A which is a two-dimensional fluid with a lattice order in the third dimension. The possibility of such a phase was

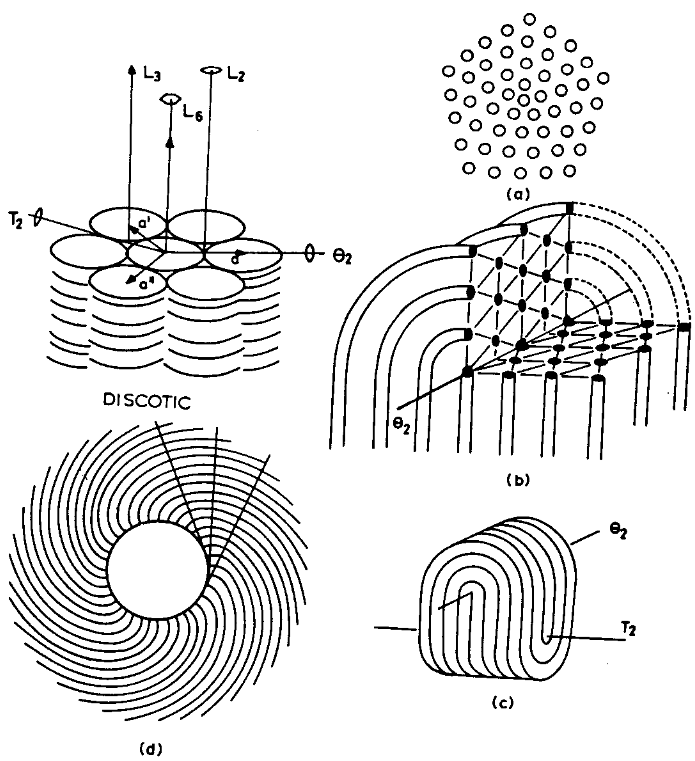

Figure 12. Symmetry elements associated with a hexagonal columnar discotic together with possible defects in these systems.

first considered from a theoretical point of view by Landau, but it was observed in thermotropic single-component systems only a decade back[21]. The structure is similar to the hexagonal phase found in lyotropic (soap-water) systems[22]. Figure 12 depicts the various symmetry elements associated with it. From this we can conclude that this phase is somewhat like the flux lattice of a type II super-conductor[23]. In fact just as in flux lattices here also we can have disclinations of strength + $N/6$ in the hexagonal lattice. In figure 12a we show one such lattice disclination of strength + 1/6. It must be remarked that the director is strictly undistorted in this defect, as it is always along the 6-fold axis. The columnar phase is also like smectic-A when looked down an orthogonal T_2 or θ_2 2-fold axis. As a consequence we can construct even smectic like + 1/2 disclinations. We show in the same figure *a* + 1/2 disclination formed about the θ_2 axis. This defect can also be connected with a similar one about T_2 axis (figure 12c). The angle between θ_2 and T_2 axes is in general a multiple of $\pi/6$. In fact the existence of such combined defects (plate 3) established the hexagonal symmetry of the lattice.

All the defects that we have constructed so far in this phase could have been easily anticipated. But this work paid rich dividends in the end. It becomes clear that one can even obtain defects of the type shown in figure 12d. Here the liquid columns are normal to the cylinder and are along involutes to it. This solution is permitted even in smectic-A. It is interesting that no one had thought of this possibility till it appeared as a natural consequence of developable domains[24,25,26].

Lattices with Biaxial Symmetry

For less symmetric structures, by and large we just get variants of the answers that we have got so

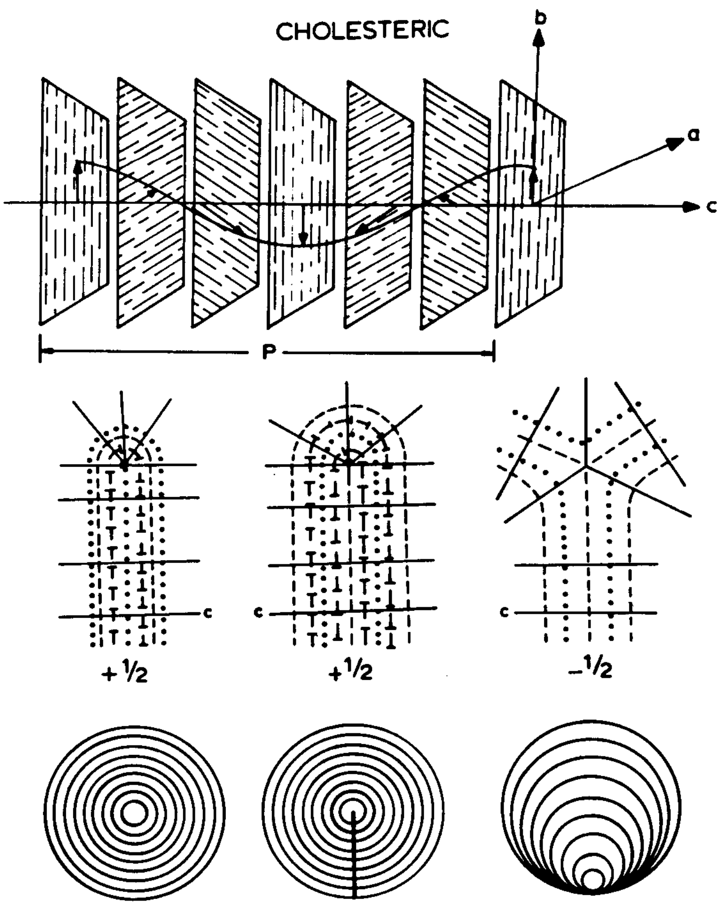

Figure 13. Line defects in cholesteric liquid crystals.

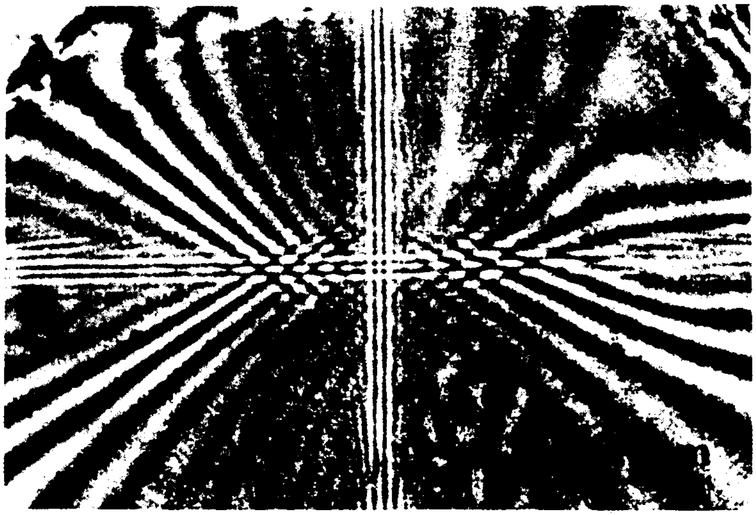

Plate 3. Combined disclinations in a columnar discotic. (After Oswald, P., *J. Phys. Lett. Paris.* **42**, L171, (1981)).

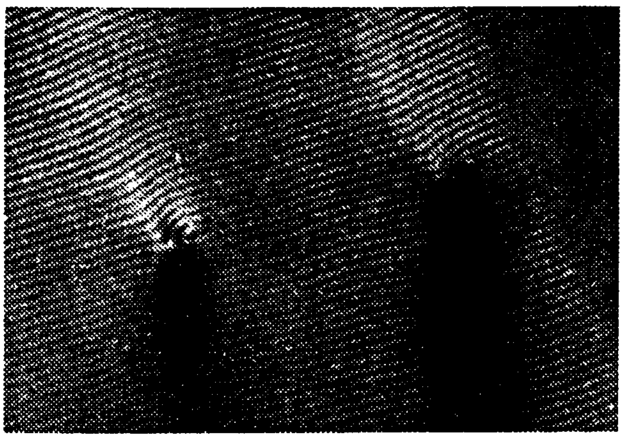

Plate 4. Edge dislocations in a cholesteric. (After Bouligand Y, *J. Phys. Paris,* **34**, 603, (1973)).

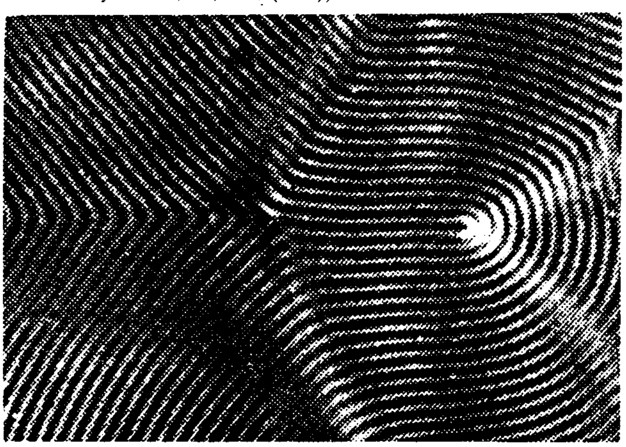

Plate 5. Pinch in a cholesteric. (After Bouligand Y, *J. Phys. Paris*, **34**, 603, (1973)).

far. But in the case of the cholesteric phase this exercise yields somewhat interesting results. It is generally looked upon as a spontaneously twisted nematic phase and also considered to be locally uniaxial about the director. However, the twist removes the local cylindrical symmetry and the structure should be looked upon as a continuously twisted biaxial phase. The three 2-fold directions at any point are respectively the twist axis, the local director and the binormal. Our experience in biaxial nematics and smectic-A can be effectively used to construct cholesteric disclinations. To bring out the special feature of cholesterics we have shown in figure 13 two $S = +1/2$ disclinations. It must be remarked that one of the half disclinations which has the director at the centre, along the disclination line was till recently considered nonsingular. But in view of twist induced biaxiality it is really singular. If this is accepted, then we get into a ticklish situation. In nematics the all circular $S = +1$ and other integral defects have twist as a part of the process that removes singularity. We may have to look upon them as singular, in the light of the above results in cholesterics.

We can even construct a Dirac monopole structure (figure 13) with the twist axis in the all radial configuration. If we insist on converting this into a Boojum then very large distortions in the cholesteric layer structure [figure 13] will be necessary. Thus it appears clear that Boojum is ruled out in cholesterics.

INTERACTION BETWEEN DISCLINATIONS: DISLOCATIONS AND PINCHES

In nematics, unlike defects can come together and finally result in a uniform state. In figure 14 we show this for line and point singularities. But this is not true for layered systems like cholesterics

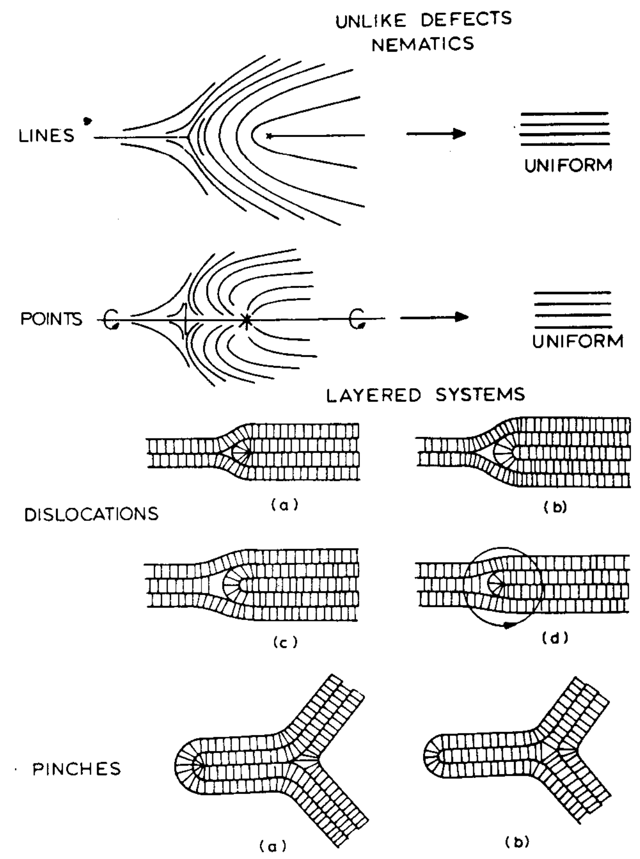

Figure 14. Interaction between unlike defects in nematics and layered systems like smectics (or cholesterics).

and smectic-A. The + 1/2 and − 1/2 of various types combine to give, surprisingly, either a dislocation or a pinch[3]. Though these defects are not easy to see in smectics they are very clearly visible in cholesterics[25,26] (see plates 4 and 5).

We can even combine like defects and get a defect of twice the strength. For Poincaré defects this exercise leads to a hedgehog when two like $S = +1/2$ structures are brought together. This is shown

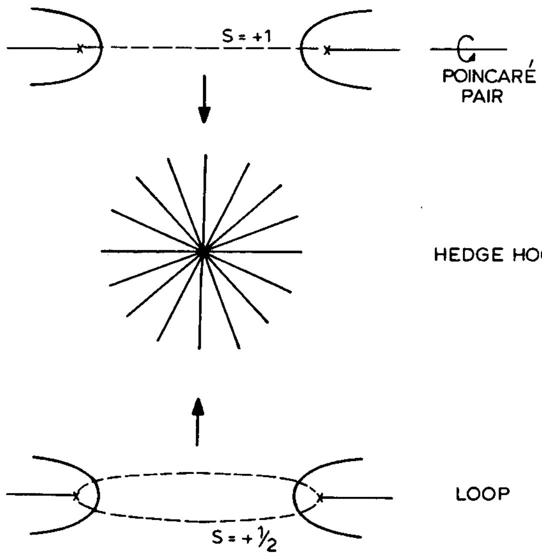

Figure 15. Two possible ways of getting a hedgehog: (1)* by combining two $S = +1/2$ Poincaré defects and (2) by the shrinking of a $S = +1/2$ disclination loop.

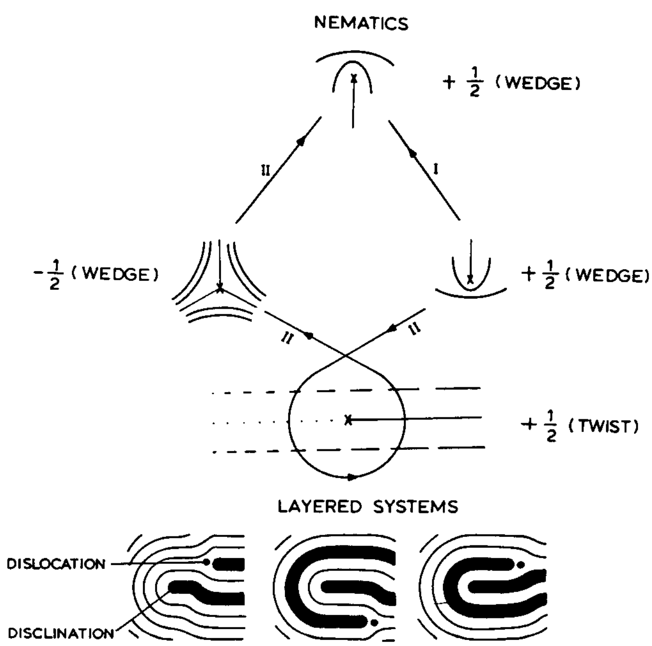

Figure 16. Effect of taking one defect round another in nematics and layered systems.

in figure 15. This particular result brings out both the strength as well as the weakness of our language. There is more than one way of getting a hedgehog. Our procedure cannot say as to which one the system will adopt. In general in many situations we get a rich class of solutions, but we cannot easily decide between them.

There is an interesting aspect[27] to the phenomenon of interaction between defects which we have diagramatically shown in figure 16. We have already seen that a nematic wedge disclination can be converted into its antidefect through a π rotation about an axis orthogonal to the disclination line. In effect this is precisely what happens when a wedge disclination is taken round a $S = 1/2$ twist disclination. In the same way a hedgehog point defect can be changed to a hyperbolic point defect by taking it round a $S = 1/2$ wedge or twist disclination. Hence when two wedge disclinations or two hedgehogs are interacting the end result for direct coalescence is different from what we get if we take one of them around a $S = 1/2$ disclination line. In biaxial nematics we find that a half disclination in one pair of fields say $a - b$ gets converted to its anti-defect when taken around a half disclination in $b - c$ or $a - c$ fields, implying again a path-dependent interaction. Even in layered systems a positive edge dislocation gets converted into a negative dislocation when taken round a $S = 1/2$ disclination (figure 16).

One important consequence of this result is that a defect of higher strength decays in the presence of $S = 1/2$ disclination line. We can understand this with an example. Let us say to start with we have a point defect of strength + 2. This can be split into two identical hedgehogs, each of strength + 1. We take one of them round the given $S = 1/2$ disclination line. Thus it gets converted to a hyperbolic point which can later on annihilate the other hedgehog on coalescence.

SOME REMARKS

We have not given all the results that we can get by these geometric arguments. We have certainly demonstrated the powers of this tool. Also this language is one of the many other ways of understanding defects in liquid crystals. The other important ones are (i) Energetics[28,29,30,31], (ii) Algebraic Topology[27], (iii) Working by analogies with defects in other branches of condensed matter physics[4,13,14]. Each language has its power as well as its limitation, and they supplement each other in our understanding of defects.

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