Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

Screw Disclinations in Nematic Samples with Cylindrical Symmetry

C. E. Williams [b a], P. E. Cladis [c a] & M. Kleman [a]

[a] Laboratoire de Physique des Solides Associé au, CNRS Université de, Paris-Sud, 91, Orsay-France

[b] Service de Physique des Solides, Centre d'Etudes Nueléaires, 91, Saclay, France

[c] Bell Laboratories, Murray Hill, New Jersey, 07974

Version of record first published: 21 Mar 2007.

To cite this article: C. E. Williams , P. E. Cladis & M. Kleman (1973): Screw Disclinations in Nematic Samples with Cylindrical Symmetry, Molecular Crystals and Liquid Crystals, 21:3-4, 355-373

To link to this article: http://dx.doi.org/10.1080/15421407308083329

Molecular Crystals and Liquid Crystals. 1973. Vol. 21, pp. 355–373

Screw Disclinations in Nematic Samples with Cylindrical Symmetry†

C. E. WILLIAMS,‡ P. E. CLADIS§ and M. KLEMAN

Laboratoire de Physique des Solides
Associé au CNRS Université de Paris-Sud
91 – Orsay – France

Received September 15, 1972

Abstract—In order to verify experimentally some recent calculations on screw disclination lines in nematics we have observed with a polarizing microscope, in a meridian section, nematic filled capillary tubes with homeotropic boundary conditions, with or without inserted fibers. In the simple case with no fiber we observe non-singular $S = +1$ lines and the point singularities associated with them. The lines of force of the directors are visualized by the flickering of the fluctuations of the molecules and correspond well to the shape predicted theoretically.

When a glass fiber (which also imposes a perpendicular orientation on the nematic) is inserted along the cylinder axis, the Frank planar solution is stable above a critical ratio r_0/R of the fiber radius to the capillary radius. This instability appears experimentally by slightly displacing the tube.

With two fibers, $S = -1$ lines are created which appear to have no singular points.

1. Introduction

Screw disclination lines in nematic liquid crystals (characterized by a rotation vector $\mathbf{\Omega}$ parallel to the line) were first described theoretically by Frank[1] on the basis of linear elasticity using the one-constant approximation, i.e. the elastic constants of splay (K_1), twist (K_2) and bend (K_3) are equal. He considered only the two-dimensional solutions for which the director lies in a plane perpendicular to the line. The molecular configuration is then described by

$$\psi = S\theta + \psi_0$$

where ψ is the angle between the director and a given axis and θ is

† Presented at the Fourth International Liquid Crystal Conference, Kent, August 21–25, 1972. Work performed under D.R.M.E., contract 71/347.

‡ Permanent address: Service de Physique des Solides, Centre d'Etudes Nucléaires, 91 – Saclay – France.

§ Present address: Bell Laboratories, Murray Hill, New Jersey 07974.

the polar angle in a plane perpendicular to the line. S† is the strength of the line and on a closed path around the line the molecules rotate by an angle $\Omega = 2\pi S$. Dzyaloshinkii[3] has shown that the same planar solutions apply when $K_1 \neq K_2 \neq K_3$ except for the $S = +1$ case where only two configurations are allowed: a radial solution where $\psi = \theta$ or a circular solution where $\psi = \theta + \pi/2$ (Fig. 1).

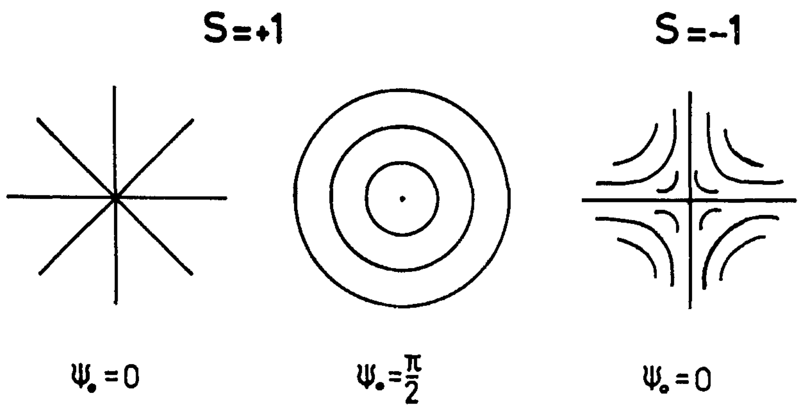

Figure 1. Molecular configuration around $S = \pm 1$ planar disclinations.

The deformation energy associated with these lines has a logarithmic divergence as r, the distance from the line, approaches zero. This necessitates the introduction of a core region, where the approximation of linear elasticity breaks down and which could be described exactly only on a molecular model. It has often been suggested that planar solutions are too restrictive and that the energy can be reduced if the core is allowed to spread throughout the sample (see Ref. 4, for instance). However detailed calculations have appeared only recently. Cladis and Kleman[5] have shown that for macroscopic samples, a non-planar, coreless solution has a lower energy than the planar solution of Frank for the $S = +1$ disclination line. This is true for any finite value of the elastic constants. Almost simultaneously Meyer[6] reached the same

† S is the index introduced by Kleman and Friedel[2]; in Frank's notation $\psi = (n/2)\theta + \psi_0$ and $n = 2S$.

conclusion for the equilibrium configuration of $S = +1$ and $S = -1$ disclinations.

In both cases the resulting director field has a radial component (case of radial solution) or an orthoradial component (case of circular solution) which decreases as $r \to 0$ but a z component which increases as $r \to 0$.

The calculations have been carried out assuming that the medium is limited to a cylinder of radius R, where the z component is zero. A simple test of the theory is therefore provided by capillary tubes containing a nematic, with homeotropic boundary conditions. This should correspond to the radial case, and $S = +1$ lines have indeed been observed with an optical polarizing microscope[6,7,8] and it has been possible to show that the equilibrium configuration is not represented by Frank's planar model but that the director has a component out of the plane which increases monotonically from the outside boundary to the center of the tube.

We report here further observations on $S = +1$ and $S = -1$ disclination lines and associated singular points.

2. Experimental Techniques

The nematic liquid crystal was MBBA (methoxy-benzilidene-butylaniline), nematic at room temperature and for which the elastic constants are known to be of the order of

$$K_1 = 5.5\ 10^{-7}\ \text{(cgs)}$$

$$K_2 = 3.5\ 10^{-7}\ \text{(cgs)}$$

$$K_3 = 8\quad 10^{-7}\ \text{(cgs)}$$

at room temperature.

The capillary tubes had a radius R between 20μ and $200\ \mu$. They were thoroughly cleaned in hot sulfochromic acid and then immersed in a solution of about 1% of hexadecyl trimethyl ammonium bromide (HTAB) in toluene so that after evaporation of the solvent a thin film was left on the surface. This film orients the molecules in homeotropic configuration (molecules perpendicular to the glass surface).

The glass fibers subsequently introduced in the tubes were subjected to the same chemical treatment.

All samples were inserted in a layer of optical epoxy resin between two parallel glass plates to avoid optical distortion due to the cylindrical shape of the glass tube. They were then observed at room temperature with a Leitz–Orthoplan polarizing microscope after the equilibrium configuration was obtained. The axis of the tube was always lying in a horizontal plane.

Two methods of observations were used:

1) Fluctuations of the extraordinary index associated with the fluctuations in orientation of the molecules which give rise to Rayleigh scattering well known in the study of light scattering in nematic liquid crystals.[9]

They are here observed in real space and, due to the large birefringence of nematic liquid crystals, are anisotropic. They appear as elongated flickering spots oriented the same way as the molecules. They are seen most clearly when one stops down the diaphragm thus increasing the depth of field and so the correlation time which becomes of the order of 1 sec.

2) Observations of a regular pattern of dots seen through the sample. Each dot gives rise to an ordinary image and an extraordinary image which may be displaced by an observable distance, depending on the position of the optical axis in the sample.[10]

The pattern of ordinary images is distorted because of the lens effect due to the cylindrical shape of the specimen; the pattern of extraordinary images is sensitive to both geometrical effects and spatial variation of anisotropy through the sample. The inclination of the displacement of the extraordinary image with respect to the ordinary image is an indication of the bend component of the director near the plane of observation i.e. the diametral plane. It has to be pointed out that our geometry is too complex to hope to get quantitative measurements by optical methods.

The pattern of dots was obtained by placing a screen across the incident beam of light in such a way that the condenser lens of the microscope forms the image of that screen on the plane of observation inside the sample.

3. Radial $S = +1$ lines

Our observations of $S = +1$ lines have been described in more detail elsewhere[7] and we shall only outline their main features here.

Rayleigh scattering was observed without an analyser and in the symmetry plane containing the axis of the cylinder. When the axis of the tube is perpendicular to the direction of polarization of the incoming light, the flickering is visible everywhere except in the middle of the sample and it shows a smooth curvature of the molecular configuration. If we rotate the sample by $\pi/2$, the flickering is apparent in the middle of the sample and directed along the tube axis.

The inclination of the displacement of the extraordinary image with respect to the ordinary image was measured and compared to the theoretically computed value of the bend angle ϕ using Cladis and Kleman's model for the anisotropic case (cf. Ref. 7, Fig. 1).

These two experimental tests are consistent with the non-singular model and show without doubt that at $r = 0$ the molecules are parallel to the direction of the " line "; as $r \rightarrow R$ it curves continuously to become perpendicular to the axis at the boundary $r = R$.

Singular points of two types were observed along the tube (Fig. 2). They are related to the fact that, for the non-planar model, two energetically equivalent configurations exist where the direction of bend is changed. As expected they alternate along the line and two consecutive points can annihilate leaving no trace. These points appear similar to the ones observed on diffused lines in bulk nematic samples between two rubbed glass plates and described in Ref. 4 (Fig. 3). It must be noticed that it is impossible to generate a line in a capillary tube without one singular point since the meniscus, where the molecules appear to be perpendicular (or almost perpendicular) to the interface, promote bending in opposite sense on each side of the tube of liquid (Fig. 2b). Very rarely the singularity is on the meniscus itself. In most cases, for short columns of nematic of the order of a few radii, the singular point appears half way through the column. It seems therefore that the direction of bending is not necessarily related to the direction of filling of the capillary tube.

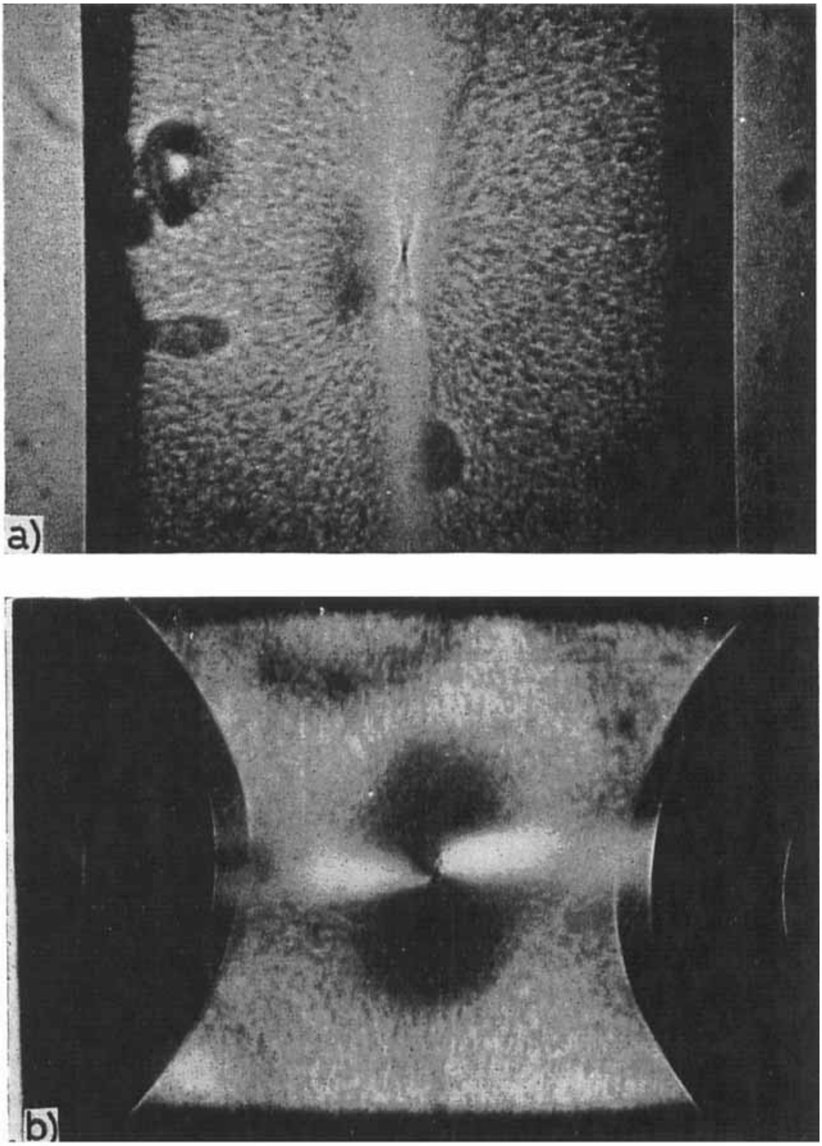

Figure 2. Singular points of two types along an $S = +1$ radial line: (b) shows the most common singular point together with the meniscus.

Figure 3. Singular points along an $S = +1$ line in a bulk sample between rubbed glass plates. The sharp line is an $S = \frac{1}{2}$.[4,6]

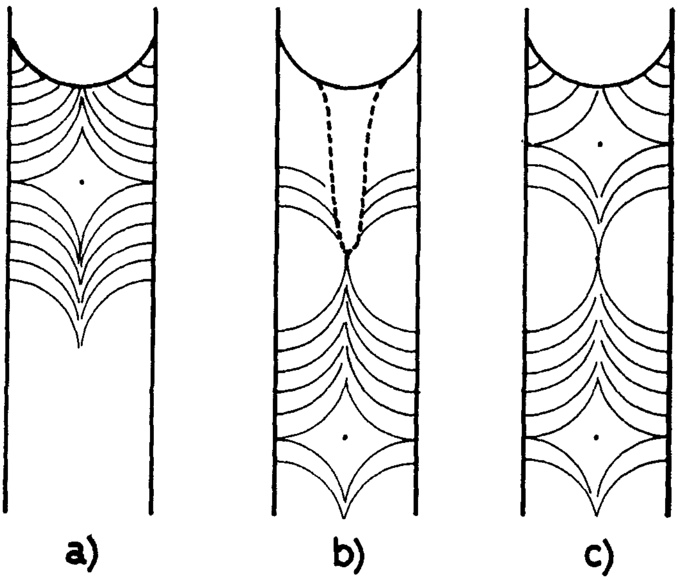

Figure 4. Schematic view of the possible mechanism by which more singular points can be created along a line by blowing slightly into the capillary tube. (a) Configuration before blowing with one singular point. (b) Apparition of a diffuse singularity (dotted line) ending with a singular point. (c) Equilibrium configuration after blowing leaving three singular points.

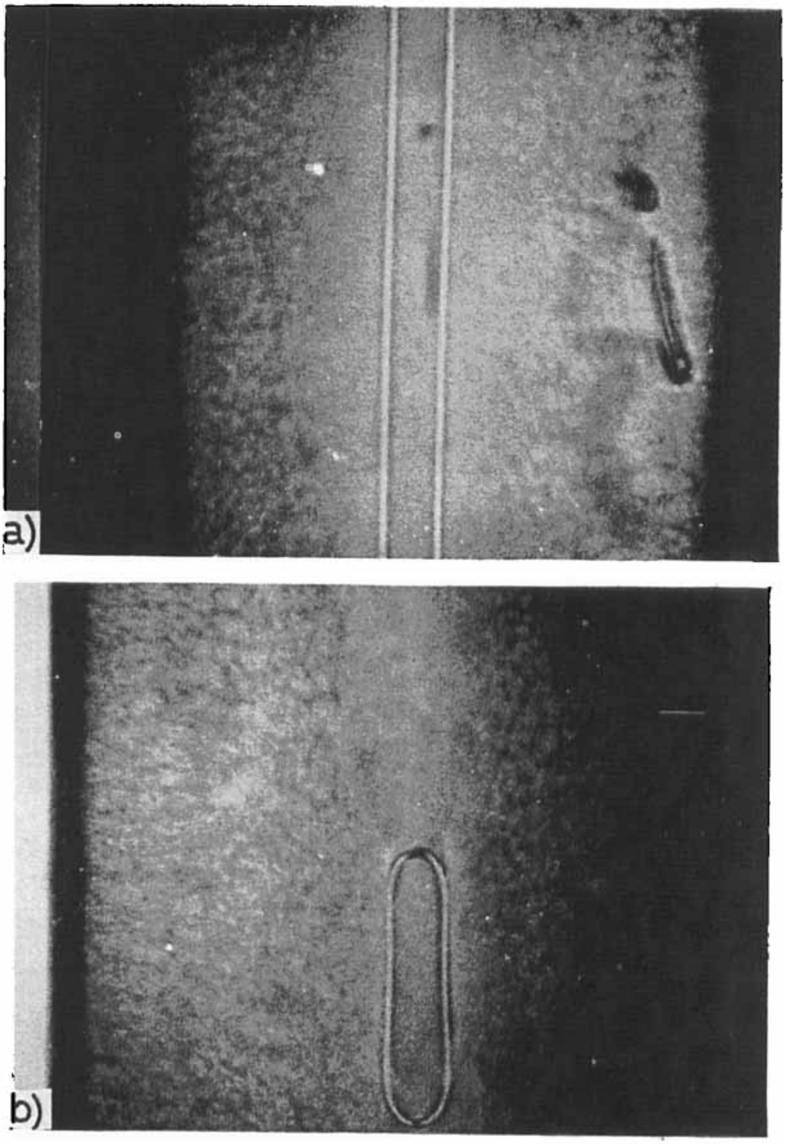

Figure 5. (a) Apparition of an optical singularity when the pressure gradient is sufficiently large. This pattern has cylindrical symmetry. (b) Relaxation of the singularity when the pressure gradient has disappeared.

It is possible to create more singular points along the line by blowing very lightly in the tube. The singular point that was present before blowing is pushed further along the tube and a singular point of the other type appears where the flow is sufficient to change the bending direction.

When there is a pressure gradient the configuration is complex and a diffuse singularity appears between the singular point and the meniscus. When the pressure gradient is released the nematic relaxes to a normal configuration but with the singular point still present. Since the meniscus imposes the reverse bending another singular point has to be formed. A possible mechanism is shown on Fig. 4.

If the pressure gradient is larger a cylindrical optical discontinuity appears along the tube. When the blowing stops, that cylinder breaks up. The loops one sees in a diametral plane have two singular points at each end and they disappear slowly leaving no trace. This feature could be of importance in flow experiment.

4. Other Configurations in the Tube

By introducing inside the capillary tube glass fibers with homeotropic boundary conditions, we were able to generate other disclination lines. The rank of those lines is obtained by noticing that each fiber introduced in the tube is equivalent to an $S = +1$ line. Since the total strength of the lines inside the tube must be equal to $+1$, as long as homeotropic conditions persist on the boundaries, we deduce that, if n is the number of fibers introduced, the total strength of the " free " lines parallel to the axis is $1 - n$.

A. Two Fibers Inserted

In that case a non-singular $S = -1$ line appears. Indeed when (Fig. 6a) the fibers are located in symmetrical positions with respect to the axis and parallel to it the flickering of light as well as the dots show a line without singular core along the axis. This seems to provide a proof for the existence of non-singular $S = -1$ lines, already proposed by J. Rault[4] and R. B. Meyer[6] (Fig. 6b). A definitive test of the model would have been to observe the change of concavity of the envelopes of the director in two perpendicular planes (these concavities, according to the model of the $S = -1$, should be in opposite direction) but it has been impossible to achieve this experiment, since any small movement given to the tube changes immediately the configuration. However the dot pattern becomes less clear if the plane containing the fibers is no longer parallel to the plane of observation which would indicate that the configuration does not have cylindrical symmetry.

We have not observed any singular points along an $S = -1$. This can be easily understood: let us consider two reverse situations like the one represented on Fig. 6b and the symmetrical one obtained by reversing the nails; their confluence along the axis would give

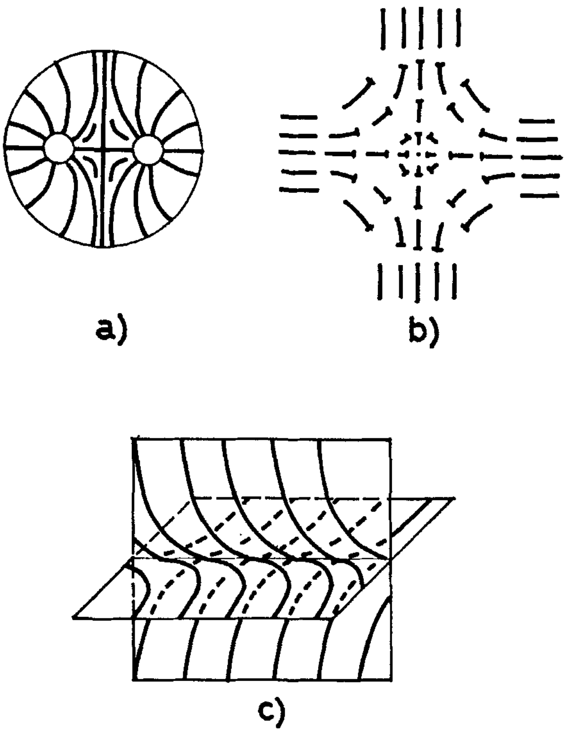

Figure 6. (a) $S = -1$ line in a capillary tube with two fibers (planar representation). (b) Detailed representation of a non-singular $S = -1$ line. (c) Envelope of the molecules in two perpendicular planes showing how the concavity is reversed.

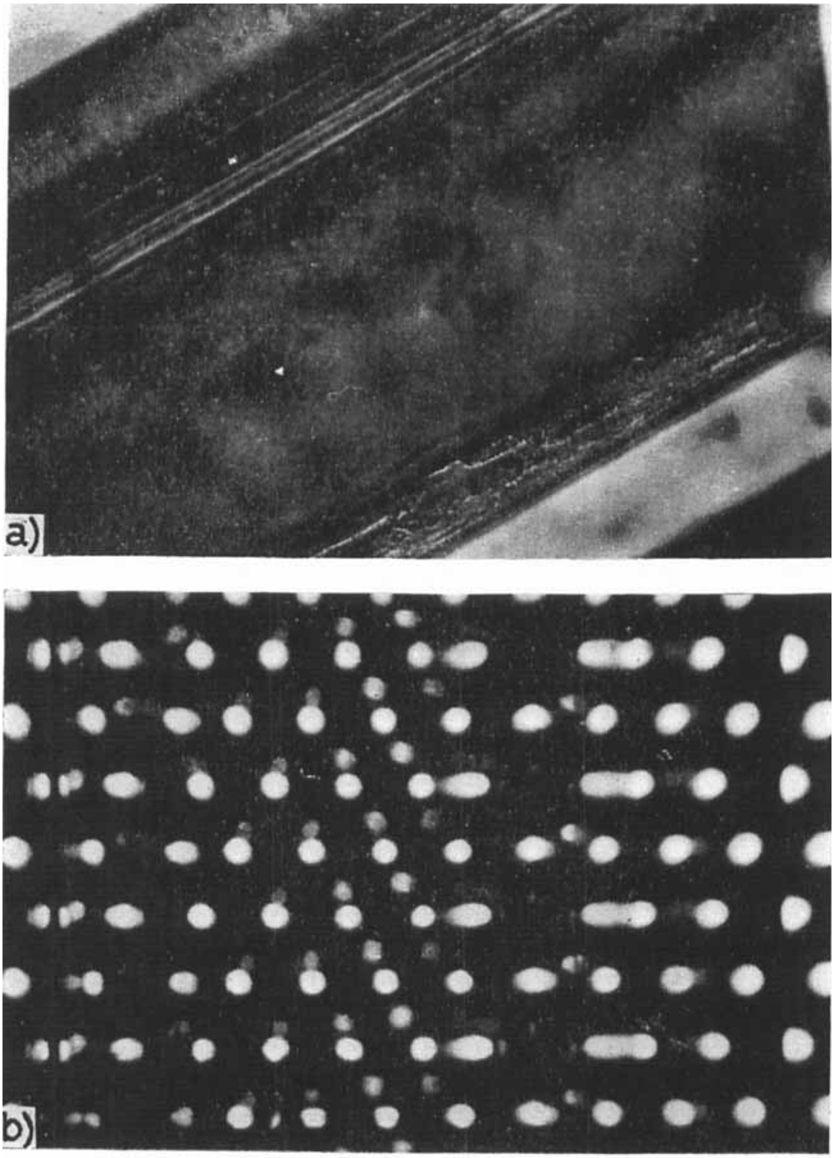

Figure 7. Capillary tubes with two fibers in a diametrical plane: (a) Rayleigh scattering; (b) Doubling of images of a dot pattern.

rise to a singular point which could disappear by a rotation of $\pi/2$ of one configuration with respect to the other one.

Figure 7 shows the aspect of the specimen with two fibers and the dots pattern showing clearly a line.

B. One Fiber Inserted

With only one fiber strictly centered along the axis, we obtain a situation which can be described as an $S = +1$, but with a core region fundamentally different from what has been described above. A theoretical discussion of this situation will provide some clues to the experimental results obtained when the fiber is approximately along the axis or displaced from that position.

B.1) *Theoretical*

We limit the discussion to the case $K = K_1 = K_2 = K_3$. Consider a tube of diameter R, and an inner fiber centered along the axis of diameter r_0. Cladis and Kleman have studied the set of solutions which correspond to homeotropic conditions on the boundary R and minimize the Frank energy density. This is schematically

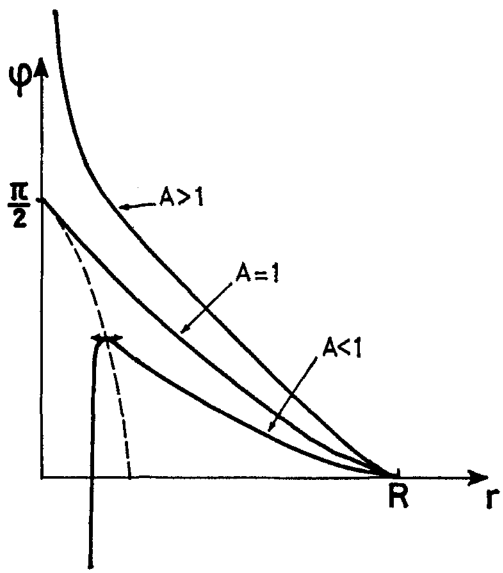

Figure 8. ϕ, angle of the director with the radial direction, versus r, distance to the axis, for different values of the constant A, after Cladis and Kleman.[5]

summarized on Fig. 8 where the angle ϕ of the director with the radial axis is plotted versus the distance r to the line axis, for different values of an integration constant A. ϕ obeys the differential equation

$$r\frac{d\phi}{dr} = \pm \sqrt{A - \sin^2 \phi}.$$

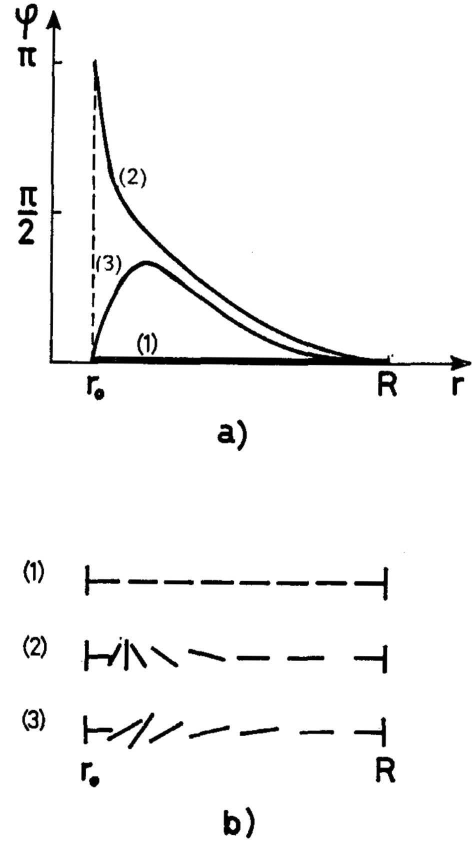

Figure 9. (a) The three possible solutions corresponding to the boundary conditions $\phi(R) = 0$ and $\phi(r_0) = 0$ or π. (The notations are the same as on Fig. 8.) Curve 1 corresponds to Frank's planar solution ($A = 0$), Curve (2), to the $A > 1$ solution and curve (3) to the $A < 1$ solution where the solution drawn on Fig. 8 has been completed in the region where it oscillates until it reaches $\phi(r_0) = 0$ for the first time. (b) Direction of the molecules in a meridian section of the cylindrical sample for the three cases considered.

Given our boundary conditions at r_0 and R, three cases occur (Fig. 9):

1) $A = 0$. This corresponds to Frank's planar solution and can evidently be achieved for any value of r_0 larger than the microscopic core radius. The energy of the nematic region is $f/\pi K = \ln R/r_0$.

2) $A < 1$, let $A = \sin^2 \alpha$. The maximum angle ϕ reached by the director is α. The curve $\phi = \phi(r)$ oscillates between values $+\alpha$ and $-\alpha$, with a periodicity decreasing exponentially as $r \to 0$.† We consider only the first oscillation where $\phi = 0$ when $r = R$, reaches its maximum value α and decreases to zero when $r = r_0$. (This is a possible solution to our problem.) For a given r_0, the angle α is given by the equation.

$$r_0/R = \exp\ -2K(\sin \alpha)$$

where $K(x)$ is the complete elliptic integral of the first kind. The energy of the nematic enclosed between the fiber and the tube boundary is

$$\frac{f}{\pi K} = 2\,|\,(2E(\sin \alpha) - \cos^2 \alpha K(\sin \alpha)\,|$$

where $E(x)$ is the complete elliptic integral of the second kind.

3) $A > 1$, let $A = 1/\sin^2 \alpha$; ϕ varies monotonically with r and the director rotates always in the same sense. If it reaches the values $\phi = \pi$ for $r = r_0$, we have the relation

$$r_0/R = \exp - 2 \sin \alpha K\,(\sin \alpha)$$

and the energy of the nematic region is

$$f/\pi K = \frac{2}{\sin \alpha}\,\{2E\,(\sin \alpha) - \cos^2 \alpha K\,(\sin \alpha)\}$$

We have to compare these three solutions. In the isotropic elasticity case here considered, the $A > 1$ solutions are always of higher energy than the $A < 1$ solutions, and the comparison could therefore be limited between $A = 0$ (Frank solution) and $A < 1$. However the experimental situation is more complex, as we shall see, and we comment successively on the stability of $A < 1$ as well as $A > 1$ solutions with respect to $A = 0$.

† In Cladis and Kleman's paper, curves corresponding to the case $A < 1$ have been considered only between $r = R$ and the first maximum. Meyer has extended these curves to the first half oscillation (as done here) to study the stability of core solutions versus the solution $A = 1$ (coreless solution).

$A = 0$ *versus* $A < 1$. According to Fig. (3), there is a limiting value of r_0 above which the only solution which exists is the Frank solution. This corresponds to a critical radius $r_c = R \exp 2K(0) = R \exp \pi$, i.e. $r_c/R \simeq 1/23$. Below that ratio, the $A < 1$ solution is always of smaller energy than the Frank solution. Above that ratio the only possible solution is the Frank planar solution. The critical energy is $f = \pi^2 K$.

On Fig. 9, we have represented the directions of the molecules in a meridian section of the tube in the case $A < 1$

$A = 0$ *versus* $A > 1$. The critical ratio r_c/R above which the Frank solution is more stable than the $A > 1$ solution is reached for a value of $\alpha \sim 65°$, i.e. $r_c/R \sim 1/69$, and the critical energy is $f \sim 4.2 \pi K$.

As shown in Fig. 9b, ϕ equals $\pi/2$ for an intermediate value r_1 of r. This value of r_1 is related to r_0 and R by the equation

$$r_0 R = r_1^2$$

B.2) *Experimental*

A perfect $A = 0$ planar solution has always been observed for well centered fibers or for sufficiently large fibers even if they were displaced from their central position in the tube (Fig. 10a and b).

However in most cases another non-singular line parallel to the axis appeared when the fiber was no longer centered. The dot pattern showed that the molecular inclination ϕ is equal to $\pi/2$ for a radius $r_1 (r_0 < r_1 < R')$ where R' is the maximum distance from the center of the fiber to the boundary of the nematic cylinder (Fig. 11a and b). This would correspond to an $A > 1$ solution.

In the region where the fiber is nearest to the tube wall the configuration is planar.

In many cases the relation $r_0 R' = r_1^2$ was verified but the ratio r_0/R did not correspond to the theoretically predicted value for having an $A > 1$ solution. However the physical situation is different from the theory since the cylindrical symmetry is not kept (fiber displaced from the center) and furthermore the elastic constants are not equal. This could account for the discrepancies.

It must be noted that the continuous transition from a planar solution on one side of the fiber to a $A > 1$ solution on the other side

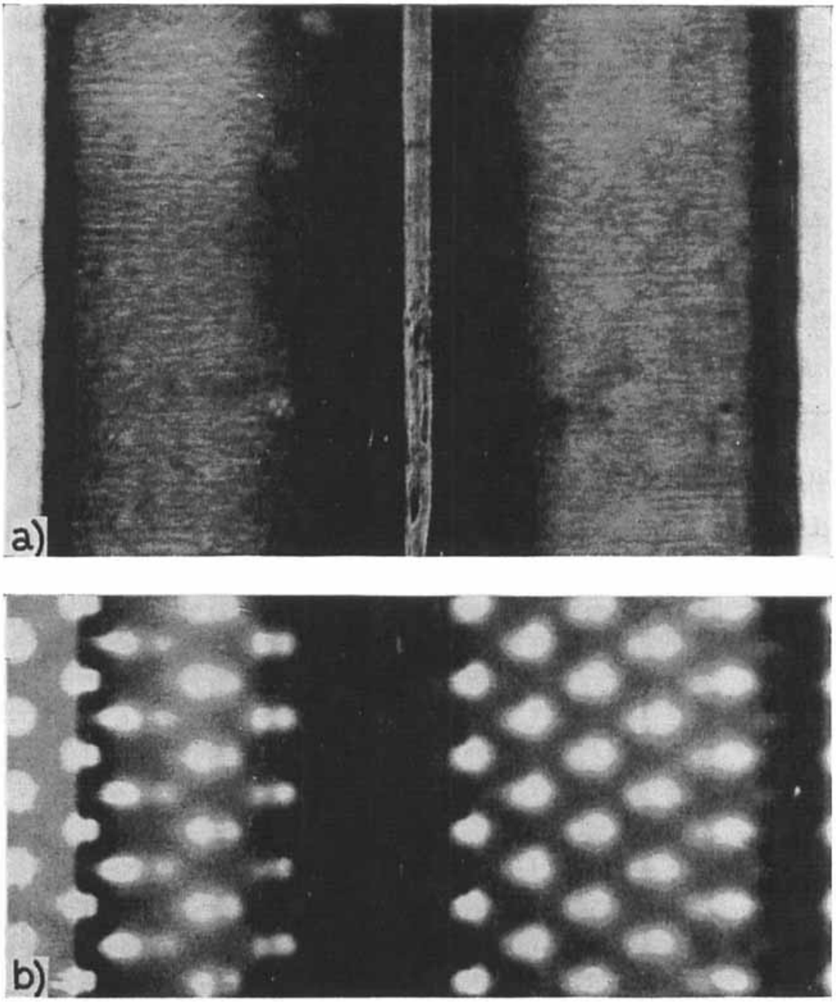

Figure 10. Planar solution in a tube with one fiber: (a) Rayleigh scattering; (b) Dot pattern.

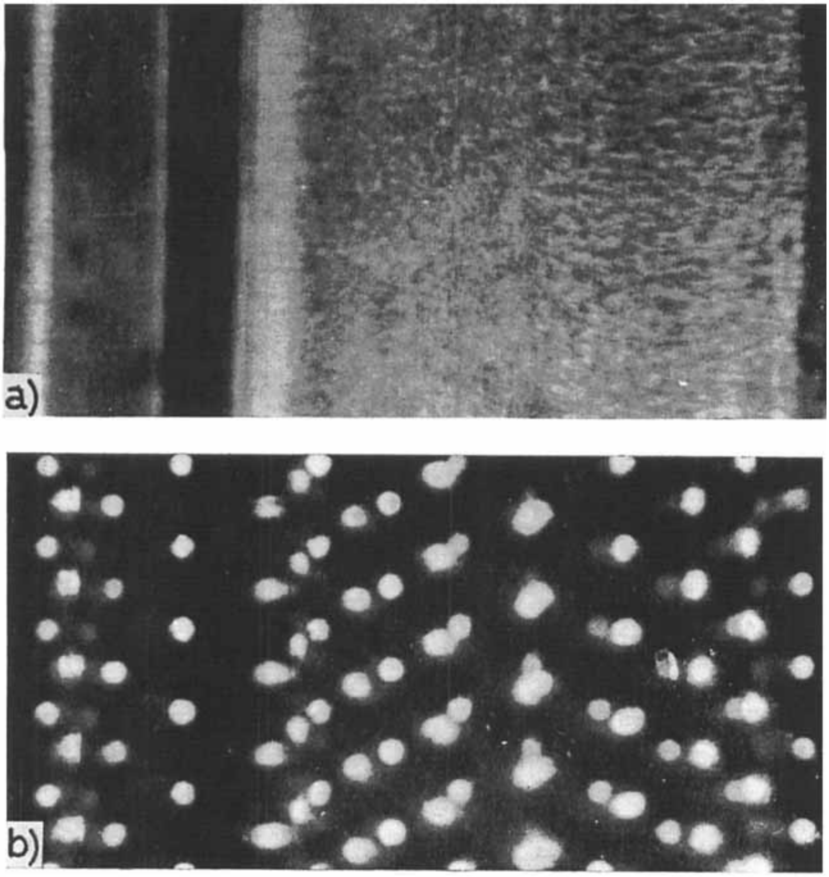

Figure 11. $A > 1$ solution in a tube with one fiber off-center: (a) Rayleigh scattering; (b) Dot pattern.

cannot be done without creating more lines which gives a more energetic overall configuration. A possibility is shown in Fig. 12 with two $S = -\frac{1}{2}$ and one extended $S = +1$. The exact location of these additional lines is not fixed and they could be difficult to observe, since one always looks at the diametral plane; however in some cases we have observed two singular lines on each side of the fiber as shown on Fig. 13. Furthermore when the two $S = -\frac{1}{2}$ lines terminate, the configuration changes and an $S = 1$ line ($A > 1$) is no longer apparent. An $A < 1$ solution should therefore start from that

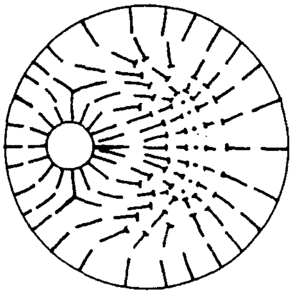

Figure 12. Possible molecular representation in a plane perpendicular to the cylinder axis with one fiber off-center showing the necessity of two $S=-\frac{1}{2}$ singular lines with the $A>1$ solution. We have assumed a coreless and extended $S=+1$ on the right part of the diagram.

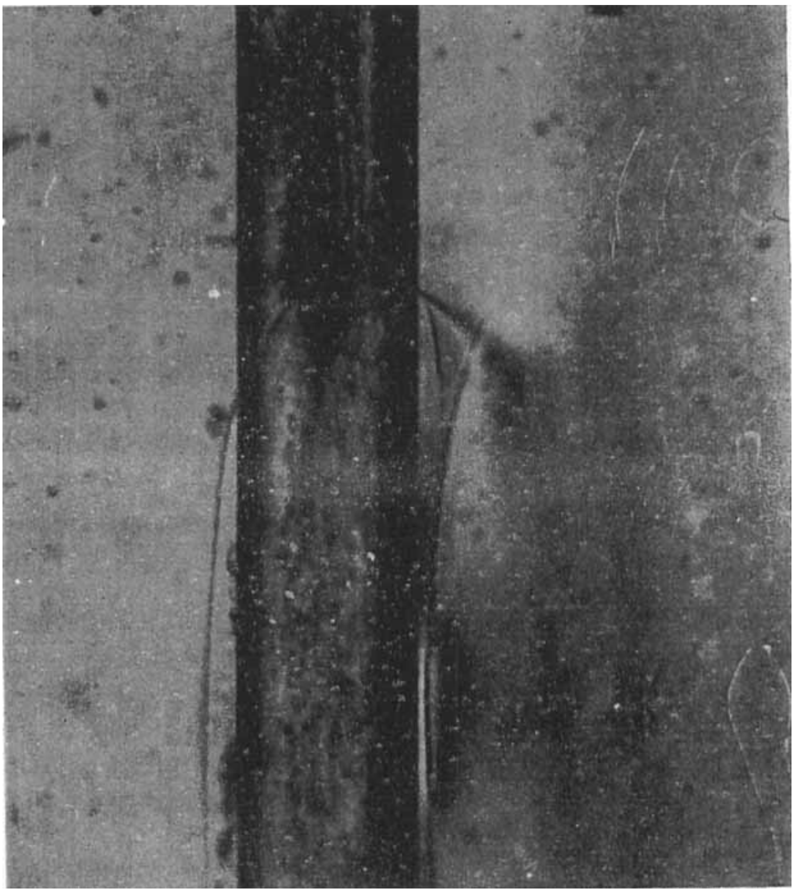

Figure 13. Photo of the two $S=\frac{1}{2}$ lines around the fiber and one $S=1$, $A>1$ line. Note that the configuration changes when the two $S=\frac{1}{2}$ lines terminate.

termination. However, let us note that the $A < 1$ solution (as deduced from the displacement of the dots), which should be the most stable solution according to the theoretical model, has been seldom observed.

Therefore the one-constant approximation ($K_1 = K_2 = K_3$) is not valid in this case and the calculations should be extended for the anisotropic case ($K_1 \neq K_2 \neq K_3$).

5. Conclusion

This experimental study shows clearly the non-singular character of cores of screw disclination lines of integer S. The director aligns parallel to the axis along the line and the spreading of the core is comparable with the dimension of the specimen.

However this is not the only possibility and the experimental situations investigated show the sensitivity of the molecular configuration around a given disclination to various boundary conditions.

These experiments also indicates that singular points along disclination lines may play an important role in flow processes.

Acknowledgements

We are grateful to Professor J. Friedel for the interest he has shown in this work.

REFERENCES

1. Frank, F. C., *Disc. Faraday Soc.* **25**, 1 (1958).
2. Kleman, M. and Friedel, J., *J. de Phys.* **30**, C-43 (1969).
3. Dzyaloshinskii, I. E., *J.E.T.P.* **31**, 773 (1970).
4. Rault, J., *J. de Phys.* **33**, 383 (1972), and *Solid State Comm.* **9**, 1965 (1971).
5. Cladis, P. E. and Kleman, M., *J. de Phys.* **33**, 591 (1972.
6. Meyer, R. B., *Phil. Mag.* **27**, 405 (1973).
7. Williams, C., Pieranski, P. and Cladis, P. E., *Phys. Rev. Letters* **29** (2), 90 (1972).
8. Scheffer, T. J. and Gruler, H., private communication.
9. De Gennes, P. G., *CRAS*, **266**, 15 (1968).
10. Grandjean, F., *Rull. Soc. Franç. Miner.* **42**, 42 (1919). For optical properties of uniaxial crystals, see for example Hartshorne, N. H. and Stuart, A., *Crystals and the Polarizing Microscope*, Edward Arnold and Company, London, 1970.