Nematic Liquid Crystals: Defects

There are two types of defects in the uniaxial nematic phase: line defects (disclinations) and point defects (hedgehogs and boojums). These are reviewed at three levels: (i) experimental observations; (ii) topological classification; and (iii) curvature elasticity. The reader is referred to the textbooks on liquid crystals (Chandrasekhar 1992, de Gennes and Prost 1993), defects (Kléman 1983), and textures (Demus and Richter 1980) for more details. More specialized texts are those in the reviews by Bouligand (1981), Chandrasekhar and Ranganath (1986), Mermin (1979), Trebin (1982), Kurik and Lavrentovich (1988), and Kléman (1989).

1. *Experimental Observations*

1.1 *Flat Nematic Slabs*

When a thick nematic sample is viewed under a microscope, the disclinations are seen as thin and thick threads, Fig. 1. Thin threads strongly scatter light and show up as sharp lines. These are true disclinations, along which the nematic symmetry of rotation is broken. The disclinations are topologically stable in the sense that no continuous deformation can transform them into a state with the uniform director field, $\mathbf{n}(\mathbf{r}) = \text{constant}$. Thin disclinations are singular in that sense that the director, that is the degeneracy parameter or phase of the order parameter of the nematic phase, is not defined along the line. Thick threads are line defects only in appearance, they are not singular disclinations. The director is smoothly curved and well defined everywhere; it can be, at least in principle, transformed into a uniform state $\mathbf{n}(\mathbf{r}) = \text{constant}$; the obstacles might be imposed by the conditions at the walls of the sample or by other defects.

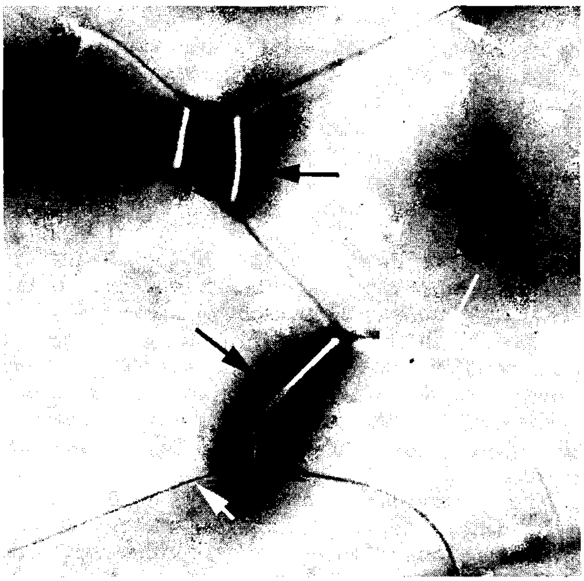


Figure 1
Thin (marked by white arrows) and thick (black arrows) threads in the nematic (*n*-pentylcyanobiphenyl (5CB)) bulk. Crossed polarizers.

In thin nematic samples (1–50 μm), the threads are often perpendicular to the bounding plates. Under a polarizing microscope, the threads show up as centers with emanating dark brushes, giving rise to the so-called Schlieren texture, Fig. 2. The dark brushes display the areas where the director $\mathbf{n}$ is either in the plane of polarization of light or in the perpendicular plane. There are usually two types of centers: with two and four dark brushes. They correspond to the thin and thick threads, respectively.

The centers with two dark bands have a sharp (singular) core, insofar as can be seen, of submicrometer dimensions and correspond to the ends of singular stable disclinations. The director rotates by an angle $\pm\pi$ when one goes around such a center. The presence of centers with two brushes signals that the director is parallel to the bounding plates: the in-plane $\pm\pi$ rotation brings the director into its equivalent state.

The centers with four brushes correspond to isolated point defects. The director undergoes a $\pm 2\pi$ rotation around the center. One can observe the difference between the two-brushes and four-brushes centers by gently shifting one of the bounding plates, Fig. 3. Upon separation in the plane of observation, the centers with two brushes leave a clear singular trace—disclination, while the centers with four brushes do not.

On rare occasions, centers with numbers of brushes higher than four are encountered. These observations signal some peculiarity of the nematic material (Madhusudana and Pratibha 1983) or of the boundary conditions (Lavrentovich and Pergamenshchik 1995).

The intensity of linearly polarized light coming through a uniform uniaxial slab depends on the angle β between the polarization direction and the optical axis (which is $\mathbf{n}$), projected onto the plane of the slab (see, e.g., Hartshorne and Stuart 1970):

$$I = I_0 \sin^2 2\beta \sin^2 \left[\frac{\pi h}{\lambda} (n_{\mathrm{e,eff}} - n_{\mathrm{o}}) \right] \tag{1}$$

where I_0 is the intensity of incident light, λ is the wavelength of light, $n_{\mathrm{e,eff}}$ is the effective refractive index that depends on the ordinary index n_{o}, extraordinary index n_{e}, and the director orientation. Equation (1) allows one to relate the number $|k|$ of director rotations by $\pm 2\pi$ around the defect core, to the number B of brushes. Since Eqn. (1) predicts that any two in-plane director orientations that differ by

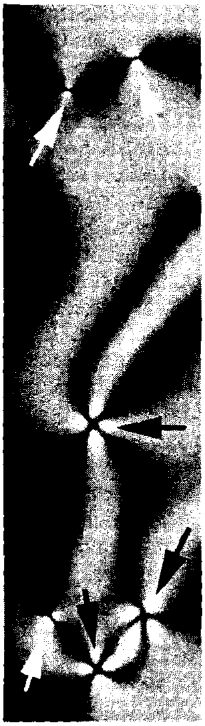


Figure 2
Schlieren texture of a thin (23 μm) slab of 5CB. Centers with two and four brushes are marked by white and black arrows, respectively. Director is in the plane of the sample. Crossed polarizers.

$\pm\pi/2$ result in the same intensity of transmitted light, then

$$|k| = \frac{B}{4} \tag{2}$$

Equation (2) is valid only when the rate of the director rotation does not change sign. In some textures, especially when the centers show more than four brushes, this restriction is not satisfied and there is no simple relationship between $|k|$ and B.

The number $|k|$ is an important characteristic of a line defect. Taken with a sign that specifies the direction of rotation, k is called the strength of disclination, and is related to a more general concept of a topological charge (but does not coincide with it).

1.2 Nematic Droplets

When left intact, textures with defects in flat samples relax into a more or less uniform state. Disclinations with positive and negative k attract each other and annihilate. However, there are situations when the equilibrium state requires topological defects. Nematic droplets suspended in an isotropic matrix such as glycerin, water, polymer, etc. (Drzaic 1995, Lavrentovich 1998), and inverted systems, such as water droplets in a nematic matrix (Poulin *et al.* 1997) are the most evident examples.

Consider a spherical nematic droplet of a radius R and the balance of the surface anchoring energy $W_a R^2$ (the coefficient is called the surface anchoring energy), and the elastic energy, KR; K is some averaged Frank elastic constant. Small droplets with $R \ll K/W_a$ avoid spatial variations of $\mathbf{n}$ at the expense of violated boundary conditions. In contrast, large droplets, $R \gg K/W_a$, satisfy boundary conditions by aligning $\mathbf{n}$ along the preferred direction(s) at the surface. Since the surface is a sphere, the result is the distorted director in the bulk, for example, a radial hedgehog when the surface orientation is normal, Fig. 4. The characteristic radius $R_c = K/W_a$ is macroscopic (microns), since $K \sim 10^{-11}$ N and $W_a \sim 10^{-5}$–10^{-6} J m^{-2}.

2. *Topological Classification*

The language of topology, or more precisely, of homotopy theory, allows one to associate the character of ordering of a medium and the types of defects arising in it, to find the laws of decay, merger, and crossing of defects, to trace out their behavior during phase transitions, etc. (Toulouse and Kléman 1976, Volovik and Mineyev 1977). The key point is occupied by the concept of topological invariant, also called a topological charge, which is inherent in every defect. The stability of the defect is guaranteed by the conservation of its charge. Homotopy classification of defects includes three steps.

First, one defines the order parameter (OP) of the system. In a nonuniform state, the OP is a function of coordinates.

Second, one determines the OP (or degeneracy) space $\mathbf{R}$, i.e., the manifold of all possible values of the OP that do not alter the thermodynamic potentials of the system. In the uniaxial nematic, $\mathbf{R}$ is a sphere denoted S^2/Z_2 with pairs of diametrically opposite points being identical. Every point of S^2/Z_2 represents a particular orientation of $\mathbf{n}$. Since $\mathbf{n} = -\mathbf{n}$, any two diametrically opposite points at S^2/Z_2 describe the same state.

The function $\mathbf{n}(\mathbf{r})$ maps the points of the nematic volume into S^2/Z_2. The mappings of interest are those of i-dimensional "spheres" enclosing defects. A line defect is enclosed by a loop, $i = 1$; a point defect is enclosed by a sphere, $i = 2$, etc.

Third, one defines the homotopy groups $\pi_i(\mathbf{R})$. The elements of these groups are mappings of i-dimensional spheres enclosing the defect in real space

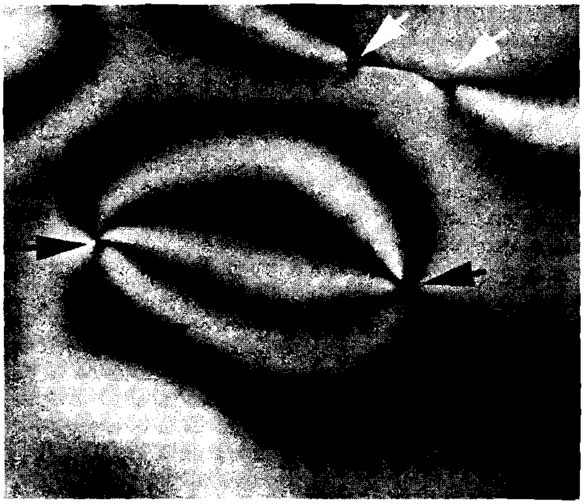


Figure 3
Shift of the upper cover plate allows one to visualize the difference between the centers with two dark brushes and four dark brushes: the former are the ends of singular lines-disclinations, while the latter are true point defects.

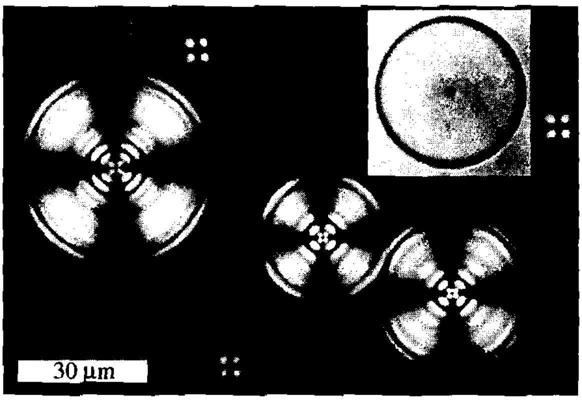


Figure 4
Polarizing-microscope texture of spherical nematic droplets suspended in glycerin doped with lecithin. The director configuration is radial and normal to the spherical surface. The insert shows the point defect-hedgehog in the center of the droplet as observed in nonpolarized light.

into the OP space. To classify the defects of dimensionality t' in a t-dimensional medium, one has to know the homotopy group $\pi_i(\mathbf{R})$ with $i = t - t' - 1$.

On the one hand, each element of $\pi_i(\mathbf{R})$ corresponds to a class of topologically stable defects; all these defects are equivalent to one another under continuous deformations. On the other hand, the elements of homotopy groups are topological charges of the defects. The defect-free state corresponds to a unit element of the homotopy group and to zero topological charge.

2.1 *Disclinations*

As an example, consider a disclination in Fig. 5 (on the left) and verify its topological stability. Let us surround the line by a loop γ that does not approach the singular region too closely (the safe distance is usually a few molecular lengths), so that $\mathbf{n}$ is well defined at every point along γ. The function $\mathbf{n}(\mathbf{r})$ maps γ into some closed contour Γ on S^2/Z_2. Γ might be of two types: (i) it starts and terminates at the same point (for example, a circle); (ii) it connects two diametrically opposite points of S^2/Z_2. Contours (i) can be continuously contracted into a single point. The corresponding director field becomes uniform, $\mathbf{n}(\mathbf{r}) =$ constant. Contours (ii) cannot be contracted: their ends remain the ends of a diameter of S^2/Z_2. Such a stable contour is shown in Fig. 5. The corresponding defect line is topologically stable. The homotopy group $\pi_1(S^2/Z_2) = Z_2 = \{0, \frac{1}{2}\}$ is composed of two elements with the addition rules $\frac{1}{2}+\frac{1}{2} = 0$ and $\frac{1}{2}+0 = \frac{1}{2}$ describing interaction of disclinations.

Thus there is only one class (with the topological invariant labeled above as $\frac{1}{2}$; in principle, one can chose any other number) of topologically stable disclinations seen in microscope as thin threads. Transformation between the classes $\frac{1}{2}$ and 0 (thick threads) is energetically impossible as it requires destruction of the nematic order at the whole half-plane ending at the line. On the other hand, all the stable lines can be continuously transformed one into another, as illustrated in Fig. 5. Although the disclinations shown on the left and on the right in Fig. 5 are usually assigned different strengths, $k = \frac{1}{2}$ and $k = -\frac{1}{2}$, the difference between them is in energy rather than in topology.

2.2 *Point Defects—Hedgehogs*

The simplest point defect is a radial hedgehog, Fig. 4. Generally, to elucidate the stability of a point defect, one encloses it by a closed surface (e.g., a sphere) σ. The function $\mathbf{n}(\mathbf{r})$ maps σ into some surface in the OP space. If this surface can be contracted to a single point, the point defect is topologically unstable. If it is wrapped N times around the sphere S^2/Z_2, the point singularity is a stable defect with a topological charge N. Since $\mathbf{n} \equiv -\mathbf{n}$, each point defect can be equally labeled by N and $-N$.

2.3 *Point Defects—Boojums*

Boojums are special point defects that, in contrast to hedgehogs, can exist only at the boundary of the

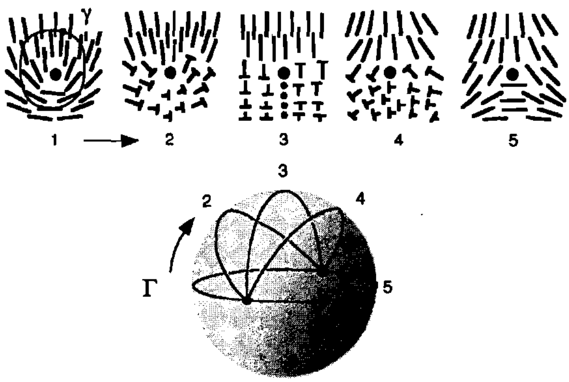


Figure 5
Stable disclinations in uniaxial nematic and corresponding contours in the order parameter space.

medium (Volovik 1978). In addition to the integer N, boojums can be characterized by a two-dimensional topological charge k of the unit vector field $\mathbf{t}$ projected by the director onto the boundary.

Point defects (both hedgehogs and boojums) in large systems such as nematic droplets with $R \gg K/W_a$, must satisfy restrictions that have their roots in the Poicaré and Gauss theorems of differential geometry:

$$\sum_i k_i = E \quad \text{and} \quad \sum_j N_j = \frac{E}{2} \tag{3}$$

Here E is the Euler characteristic of boundary. For a sphere $E = 2$ and for a torus $E = 0$. Figure 4 illustrates the simplest example with $N = 2/2 = 1$.

3. *Energetics of Defects*

The relative stability of stable disclinations depends on the Frank elastic constants of splay (K_{11}), twist (K_{22}), bend (K_{33}) and saddle-splay (K_{24}) in the Frank-Oseen elastic free energy density functional; the role of the elastic constant K_{13} in the structure of defects is not clarified yet.

Frank (1958) considered planar disclinations with $\mathbf{n}$ perpendicular to the line. In this case, the K_{24}-term in the line's energy is zero. In the approximation $K_{11} = K_{22} = K_{33} = K$, the equilibrium director configuration around the line writes

$$\mathbf{n} = \{\cos(k\varphi + c), \sin(k\varphi + c), 0\} \tag{4}$$

where $\varphi = \tan^{-1}(y/x)$, x and y are Cartesian coordinates normal to the line, c is a constant; and another constant k is the familiar integer or semi-integer number, the strength of disclination, that shows the number of rotations of the director around the line.

The energy per unit length (line tension) of a planar disclination is

$$F_{11} = \pi K k^2 \ln \frac{L}{r_c} + F_c \tag{5}$$

where L is the characteristic size of the system, r_c and F_c are respectively the radius and the energy of the disclination core, a region in which the distortions are too strong to be described by a phenomenological theory.

The Frank theory does not distinguish lines of integer and semi-integer strength, except for the fact that the lines with $|k| = 1$ tend to split into pairs of lines $|k| = 1/2$, which reduces the energy, according to Eqn (5). The lines of integer k, as already discussed, are fundamentally unstable. Imagine a circular cylinder with normal orientation of $\mathbf{n}$ at the boundaries, Fig. 6(a). The planar disclination would have a radial-like director field normal to the axis of the cylinder, $k = 1$. However, the director can be reoriented along the axis. This "escape in the third dimension," is energetically favorable, since the energy of the escaped configuration is only $3\pi K$ (Cladis and Kléman 1972, Meyer 1973). When opposite directions of the escape meet, a point defect-hedgehog is formed, Fig. 6(b). Anisimov and Dzyaloshinskii 1972 showed that, in additional to planar lines, bulk disclinations can exist, in which the director does not lie in a single plane.

Unlike point defects such as vacancies in solids, topological point defects in nematics cause disturbances over the whole volume. The curvature energy of the point defect is proportional to the size R of the system. For example,

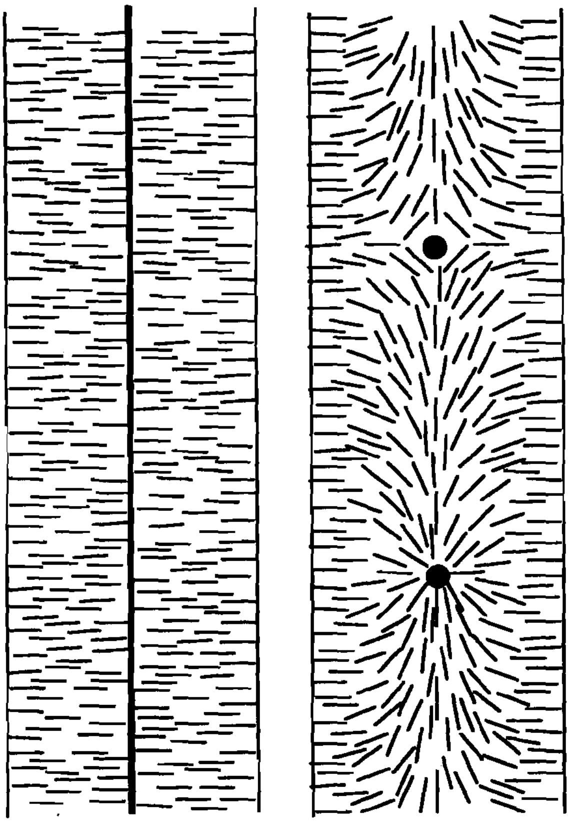
$$F_{\text{rh}} = 8\pi R(K_{11} - K_{24}) + F_{\text{cr}}$$

and

$$F_{\text{hh}} = 8\pi R\left(\frac{K_{11}}{5} + \frac{2K_{33}}{15} + \frac{K_{24}}{3}\right) + F_{\text{ch}},$$

for the radial hedgehog with $\mathbf{n} = (x, y, z)/\sqrt{x^2+y^2+z^2}$, and the hyperbolic hedgehog with $\mathbf{n} = (-x, -y, z)/\sqrt{x^2+y^2+z^2}$, respectively.

There are still many open questions concerning the behavior of defects in shear flows, external fields, and their dynamics and interaction. Note that the classification of defects in biaxial nematics is drastically different from that in the uniaxial nematics considered above. In the biaxial nematics, there are no hedgehogs (although boojums are allowed), and there are five topological classes of disclinations (Toulouse 1977). It turns out that both $|k| = n/2$ and $|k| = n$ are stable disclinations; those with $|k| = 2n$ are not; here n is an integer. Some pairs of disclinations cannot cross each other without creation of a third disclination that joins the original pair. Other distinctive features are expected in energetics: since the line tension scales as k^2, singular lines $|k| = n$ should tend to split into lines



(a) (b)

Figure 6
Singular disclination of strength $k = 1$ in a cylindrical capillary (a) escapes in the third dimension creating point defect-hedgehogs (b).

$|k| = n/2$. Both topology and energetics of disclinations might actually help to clarify the status of biaxial nematics.

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