Defects in Nematic Liquid Crystals

Seminar

Miha Ravnik
Adviser: Professor Slobodan Žumer

Defects in liquid crystals are discontinuities in order parameter. In nematic liquid crystals (NLC) two types of stable defects exist: disclination lines and point defects. Defects formation depends on isotropic to nematic phase transition while their stability depends strongly on confining surface properties, surface geometry and presence of external field. Classical Frank’s model of director elasticity is unable to describe core of the defects, therefore core radius and core free energy must be introduced. In experimental studies of defects typically two techniques are mostly used: polarization microscopy and fluorescence confocal polarizing microscopy.

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1. Introduction

Defects in nematic liquid crystals (NLCs) are topological objects related to discontinuous average orientation of constituent molecules \[1\]. Their behaviour and size is different as in solid state (crystalline) samples due to the “softness” of liquid crystals and long-range influence of boundary surfaces. In solid state samples defects are typically of atomic scale (~Å) and their influence on surrounding media is highly localized. Liquid crystal defects are on the other hand of at least two magnitude larger scale (molecule scale \(~100\)Å) and they determine the behaviour of the whole NLC sample. Larger scale of defects in NLC consequently enables simpler techniques for defects creation and study.

Nematic liquid crystals are fluids that possess orientational but no positional order. They are made of organic molecules with strongly anisometric shape \[2\], \[3\]. The direction of local orientation is determined by the director \(\mathbf{n}\), which changes in space. Director is therefore in general not only a vector but a vector field \(\mathbf{n} = \mathbf{n}(\mathbf{r})\), where \(\mathbf{r}\) is position vector in coordinate space. The basic property of director field is that director stetes \(\mathbf{n}\) and \(-\mathbf{n}\) are indistinguishably; this is called \(\mathbf{n} \rightarrow -\mathbf{n}\) symmetry. There are no long range correlations in the molecular positions, but still the nematic fluid has anisotropic properties, like a true crystal. From the optical standpoint, a uniformly oriented nematic is equivalent to uniaxial monocrystal with the director being its optical axis. Schematic presentation of calamitic NLCs is shown in Figure 1. When the boundary conditions or external field do not permit uniform orientation, the solution of minimum free energy can exhibit singularities; these singularity points or lines are called defects or disclinations.

Due to fluidity and long range influence of boundary conditions, defects in NLC exhibit many interesting phenomena. Of particular interest are annihilation of defects with antidefects, defects correlations, stability and instability, role of geometry and properties of boundary surfaces on formation of defects, etc. In NLCs there are two major types of defects: one dimensional line defects and zero dimensional point defects \[3\]. Two dimensional defects, known also as walls, are not stable (without external field). Schematic picture of the radial point defect is presented in Figure 2.

Defects in LC can be within topological theory of defects described as topological objects \[4\]. Inhomogeneous vector field contains topological defects if by no continuous variation of vector field inhomogeneity can be eliminated. Every defect is characterised with its topological charge (strength), which is conserved in any variation of vector field. Transformations and combining (dynamics) of defects with equal dimensionality is...
topologically described with homotopic groups of different order, depending on the defect and studied space dimensionality.

Two main techniques have been developed for experimental study of defects in liquid crystals: polarization microscopy (PM) and fluorescent confocal microscopy (FCM). In both techniques samples are illuminated with light (polarized or nonpolarized) and intensity of transmitted (PM) or reflected (FCM) light is measured. Both methods will be described more in details in Section 3. A schematic picture of NLC defects taken with polarization microscopy technique is presented in Figure 3.

Study of defects is also a highly interdisciplinary area of physics [5]. Analogies with liquid crystal (LC) defects have been confirmed for some magnetic, superconducting and superfluid systems. But the most extraordinary analogy of LC defects is the description of early Universe by Kibble’s mechanism [5].

2. Defects in Nematic Liquid Crystals

2.1 “Origin” - Formation of Defects at Nematic to Isotropic Phase Transition

NLCs possess minimum free energy in nematic phase when all molecules are on average aligned uniformly along one preferred direction in space. If nematic sample is heated into the isotropic phase uniformity breaks and in equilibrium molecules are orientated randomly. However, if we were to look closely enough at the molecules, we would see that, locally, their orientations are correlated. This order persists over a certain characteristic distance, called the coherence length [3].

Isotropic to nematic phase transitions are favoured by the formation of defects. Thermal fluctuations are present in all LC samples and as mentioned above local order over the coherence length exist. Therefore when starting with a sample in isotropic phase and cooling it into nematic phase initial deviations from absolute isotropic phase are enhanced [6]. Stable or unstable defects are formed. Stability of defects depends strongly on boundary surface properties, surface geometry and external field. With suitable surface or field unstable defects can be stabilized and vice versa. Schematic picture of radial defect formation is presented in Figure 4.

2.2 Surface

Description and properties of LC defects depend strongly on surface properties of the studied system [3]. In experiments samples are usually prepared by confining nematic fluid between glass plates. For study of defects glass plates are polished in various directions or dirtied in periodic or totally coincidental way. Initial alignment along boundary surfaces in NLC is reflected in orientation of the NLC sample as a whole. This behaviour is totally
different in crystalline or other solid samples, where boundary surfaces are of little importance.

An important type of surface-to-NLCs interaction is the anchoring phenomenon, where surface tension depends on the director orientation [4]. For simple modelling of anchoring phenomena we presume that there exists an equilibrium orientation of director, called “easy axis”, which is prescribed by the surface properties. In experiments two easy axes are typically used. If easy axis lies in surface plane, surface imposes “planar” boundary condition, if easy axis is perpendicular to the surface plane the boundary condition is called “homeotropic”.

2.3 Disclination Lines and Point Defects

As already mentioned, two types of stable defects exist in uniaxial NLC: disclination lines and point defects. There is a topological difference between line defects and point defects (different dimensionality) therefore let us separately describe each one of them.

2.3.1 Disclination Lines

Term disclination line is used for line defects along which the symmetry of rotation is broken [4]. The director field is everywhere continuous, except on disclination line. Disclination line can be absolutely described by the “strength” of disclination \( k \), which is also preserved in different dynamic processes (e.g. annihilation). Strength of disclination is always of integer or half-integer value.

\[
k = \pm \frac{1}{2}, \pm 1, \pm \frac{3}{2}, \ldots,
\]

Strength of disclination has a very representative meaning. Its definition is as ratio \( k = \alpha / 2\pi \), where \( \alpha \) is the angle by which the director rotates after the traversal of circle surrounding the disclination line [4]. The sign of \( \alpha \) is determined by the comparison of travelling direction along the surrounding circle and direction of director rotation, when travelling along the circle. If directions are opposite \( \alpha \) is negative, otherwise \( \alpha \) is positive. Schematic picture of strength and sign determination is presented in Figure 5.

From phenomenological point of view disclinations can be described as elastic distortions of director field around the disclination line [4]. This representation is valid in whole coordinate space except in the core of the disclination line, where director field is discontinuous. Therefore we introduce the core radius of the disclination line, \( r_c \), which is in real samples is of the size of a constituent molecule, and the core free energy \( f_c \), which represents the energy of the core. Free energy volume density \( f \) in Frank’s model can be written as:

\[
f = \begin{cases} 
\frac{1}{2}K_1 (\text{div}(\vec{n}))^2 + \frac{1}{2}K_2 (\vec{n} \cdot \text{rot}(\vec{n}))^2 + \frac{1}{2}K_3 (\vec{n} \times \text{rot}(\vec{n}))^2, & \text{outside the core} \\
f_c, & \text{inside the core}
\end{cases}
\]

where \( K_1, K_2, K_3 \) are material constants describing three possible director variations in space: splay, twist, bend.

In real samples two types of disclination lines exist: the wedge disclination lines (WDL) and twist disclination lines (TDL). WDL are lines around which director field changes only by splay and bend, while director field surrounding TDL changes only by the twist.
Because the twist is always three dimensional changing, while splay and twist can also be only two dimensional, theoretical models describing TDL and WDL are also three and two dimensional.

Director orientation around wedge disclination lines with different strength are shown in Figure 6.

Figure 6: Director configuration around wedge disclination lines of different strength $k$. Disclination lines are perpendicular to the sheet and lie in centres of squares. [4]

Wedge disclination lines are usually described by planar model introduced by Frank, under the assumption $K_1 = K_3 = K$ [4]. The director field can be written as:

$$\vec{n}(x, y, z) = (\cos \phi(x, y), \sin \phi(x, y), 0).$$

(1.3)

Note that polar angle $\phi$ is a function of Cartesian coordinates. Using Euler-Lagrange equations we get:

$$\Delta \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0.$$

(1.4)

Using expressions (1.3), (1.4) and assumptions $K_1 = K_3 = K$, $K_2 = 0$ it can be shown that free energy volume density (1.2) rewrites into:

$$f = \frac{1}{2} K (\nabla \phi)^2.$$

(1.5)
Integrating equation (1.5) by plane and using singular solution of (1.4) we get elastic free energy per unit length of line $\tilde{F}$:

$$\tilde{F} = \pi Kk^2 \ln \frac{R}{r_C} + \tilde{F}_c,$$

where $\tilde{F}_c$ is core free energy per unit length of line and $R$ represents distance between WDL and the walls of container, or the distance to other disclinations. Typical values for the “$\ln()$” factor are $\sim 10$.

As already mentioned this model can not describe the details in the core. Other approaches, e.g. Ginzburg-Landau theory [4], should be used. But still this model yields an important result: the instability of WDL of integer strength. Due to coefficient $k^2$ in (1.6) out-of-core free energy of WDL lines with strength $k = \pm 1$ will be two times higher than the sum of free energies of two $k = \pm 1/2$ lines. Disclination lines with integer strength will therefore split into half-integer strength lines. Note that this behaviour derives from the simplest (Frank’s) model and does not describe real behaviour when boundary effects (e.g. tangential boundary condition) become of importance.

Twist disclinations are favoured when twist material constant $K_2$ is smaller than splay or bend material constants. A typical director orientation along TDL is when LC molecules form a Möbius strip. These types of disclinations usually appear in smectic liquid crystals, which are currently not of our interest.

2.3.2 Point Defects

Point defects form either in the bulk or at the surfaces [2]. They are only of integer strength $k = \pm 1, \pm 2, \pm 3, \ldots$ [7]. Stability and even formation of defects, as already mentioned, depends strongly on boundary surface, which in general can impose very complicate director field. Therefore in theoretical models usually only systems with highly symmetrical boundary surfaces are studied, e.g. in cylindrical or in spherical geometry. Typical defect in a sphere is presented in Figure 7.

For calculation of free energy as by disclination lines Frank’s model is used [4]. The free energy density function is again discontinuous in point defects, therefore core radius and core free energy $F_c$ again must be introduced to avoid nonphysical solutions. For the simplest radial point defect (see Figure 7) calculation of elastic free energy $F$ in one constant approximation yields:

$$F = K \left( R - \frac{2r_C}{3} \right) + F_c,$$

where $R$ again represents distance between point defect and the walls of the container or the distance to other defects. Note that typically $R \gg r_C$ and therefore core contribution in (1.7) can be neglected. This is an important difference in comparison to disclination lines where $r_C$ could not have been neglected due to singularity of free energy line density $\tilde{F}$ (1.6) in core.

2.3.3 Disclination Core

Disclination core is a region around a disclination line or point defect, where gradient of director field is large on molecular size scale and Frank’s theory (see equation (1.2)) fails [1]. Typical diameter of disclination core is one or two molecular lengths (~50Å). Due to small length scales experimental studies of disclination cores are difficult and until now only
studies with tobacco mosaic virus (TMV) molecules (TMV molecules are much larger than typical LC molecules) along wedge disclination lines have been made. Experiment has shown that TMV molecules orientate along disclination line. But it is not known whether this observations are unique to TMV, or are more general [1].

Two models of disclination core should be mentioned. First one proposes isotropic orientation in core - “melt-down”. In isotropic model core radius can be estimated by continuity condition of total free energy density \( f_{tot} \) on core surface. Elastic free energy outside the core is scaled as \( f_{el} \sim K/r^2 \). Total free energy density can be in Landau’s model constructed as:

\[
 f_{tot} = \begin{cases} 
 f_c + \frac{a}{2} (T - T^*) S^2 + \frac{b}{4} S^4 + \frac{K}{r^2}, & \text{outside the core} \\
 f_c, & \text{inside the core}
\end{cases}
\]

where \( T \) is temperature, \( T^* \) is temperature parameter of nematic to isotropic phase transition and is typically 1K lower than the temperature of isotropic to nematic transition, \( a \) and \( b \) are positive constants and \( S \) is order parameter which measures the degree of molecules orientated along director. In general \( S \) is tensor of rang 4. For isotropic samples \( S = 0 \) and for uniaxial samples \( S \approx 1 \). Elastic constant \( K \) is proportional to \( S^2 \), therefore it can be written: \( K = LS^2 \).

Using continuity condition and neglecting \( bS^4/4 \) due to \( a(T - T^*)S^2/2 \gg bS^4/4 \) we get:

\[
 r_c \sim \sqrt{\frac{2L}{a(T^* - T)}}.
\]

Note that the core radius raises with \( T \) approaching \( T^* \) and spreads over whole space when sample reaches isotropic phase.

Second model (Landau - de Gennes) in based on order parameter tensor variation. In contrast to isotropic core model it suggests strong biaxiality and predicts oblate molecular distribution along disclinations. Free energy density in this model is continuous also in core region, therefore core radius and core free energy introduction is not needed. Schematic picture of biaxial core structure is presented in Figure 8.

3. Measurement Techniques

Microscopy techniques with polarized or nonpolarized light are typically used to measure orientation of director field and consequentially position and type of LC defects. In classical technique the measured quantity is the refractive index, which varies in space due to different orientation of LC molecules. Second technique developed in recent years uses a new approach of adding fluorescence light emitting dye into nematic samples. We will separately describe both mentioned techniques: classical polarization microscopy (PM) and fluorescence confocal microscopy (FCM).

The simplest nematic LC samples are uniaxial, with their optic axis oriented along the director. The optic axis is by definition direction in optic material along which refractive index for nonpolarized light is constant [8]. However, for any other direction birefringence appears. When a light ray enters in general direction in the birefringive material it splits in two rays, ordinary and
extraordinary, with perpendicular polarization. This happens due to anisotropy of refractive index, the direction dependence of which in uniaxial samples can be presented as a rotational ellipsoid (see Figure 9). Its longer axis is called extraordinary refractive index $n_e$ and shorter axis the ordinary refractive index $n_o$. In LC samples refractive indices are typically $n_o \sim 1.5$ and $n_e \sim 1.7$.

### 3.1 Polarization Microscopy

Polarization microscopy uses birefringence properties of LC samples. Nematic slab is typically sandwiched between two glass plates and placed between two crossed polarizers [4]. Schematic picture of polarization microscopy experiment is shown in Figure 10, quantities needed for determination of transmitted light intensity are presented in Figure 11.

![Figure 10: Schematic picture of polarization microscopy experiment [8].](image1)

![Figure 11: Schematic picture of experiment with angle $\beta$ between planar dependent director and incident light polarization [4].](image2)

With classical polarization microscopy only “2D” samples with director confined in one plane are studied (director can make also constant angle to z axis). It is therefore assumed that director depends only on in-plane coordinates $(x,y)$ (see Figure 11). Monochromatic light beam usually impinges along z axis and when passing first polarizer becomes linearly polarized [4]. Then light beam “entering” into nematic sample due to birefringence splits into ordinary and extraordinary wave, each travelling with different speed (different refractive indices). Phase shift between ordinary and extraordinary wave is gained. Light leaving nematic sample is therefore cylindrically polarized. When passing through analyser again only polarization along transmission direction is transmitted. Considering all this effects intensity of transmitted light $I$ can be written [4]:

$$I(x, y) = I_0 \sin^2(2\beta(x, y))\sin^2 \left( \frac{\pi d}{\lambda_0}(n_e - n_o) \right), \quad (1.10)$$

where $I_0$ is intensity of incident light, $\beta$ is planar dependent angle between incident polarization and planar dependent director, $d$ is thickness of the nematic sample and $\lambda_0$ is the wavelength of incident light in vacuum.

Equation (1.10) is the basic formula which enables the interpretation of light textures seen when light passes the analyser. The most important term in (1.10) is the dependence of transmitted intensity on $\beta$. Note that when director is parallel to either polarizer or analyser, transmitted intensity is zero; dark region would be seen. Due to varying director field in
sample various textures (Schlieren textures) of black brushes and defects can be seen. Schlieren textures can be “read” in following way: spots where two black brushes meet are the ends of disclination lines and spots where four dark brushes meet are the cores of point defects. Schlieren texture with corresponding microscopic orientation of molecules is presented in Figure 12.

![Schlieren texture of a thin (~1 µm) uniaxial nematic](image)

**Figure 12:** Schlieren texture of a thin (~1 µm) uniaxial nematic (a) with corresponding schematic picture of director orientation (b). In picture (a) also an unstable wall defect is visible (black arrow) [4].

### 3.2 Fluorescence Confocal Microscopy

The main advantage of fluorescence confocal microscopy (FCM) in comparison to classical polarized microscopy is that three dimensional imaging of director orientation, consequently three dimensional imaging of LC defects can be made and that it has better spatial resolution [6]. In FCM experiments inspected specimens are doped with a high-quantum-yield fluorescence dye that strongly absorbs light of

![Fluorescence Confocal Microscopy](image)

**Figure 13:** General optical scheme of a fluorescence confocal microscope [6]

![Fluorescence Confocal Microscopy](image)

**Figure 14:** Picture of wedge disclination in cholesteric LC taken with FCM apparatus: (a) in plane of the sample, (b) in the vertical cross-section, along line indicated in part a, (c) variation of director

![Fluorescence Confocal Microscopy](image)
appropriate wavelength (typically laser-light) [6]. Emitted light is then studied. Fluorescence dye molecules must be of approximately the same size and shape as nematic molecules, so that they can order along with nematics [2]. Excited dye molecules fluoresce at somewhat longer wavelength (lower energies) than that of incident light. If the difference between the fluorescence and incident wavelength (Stokes shift) is sufficiently large intensities of both wavelengths can be separately detected. If the specimen is heterogeneous (non-uniform director field) dye concentration is coordinate-dependent and a high contrast image can be taken.

Three dimensional imaging is achieved with optical system of lenses (objective) that focuses incident light in a small voxel (“3D pixel”) of submicronic size [6]. Horizontal screening (see Figure 13) is typically performed by optical scanning, while mechanical refocusing at different depth is used in horizontal direction. Schematic picture of fluorescence confocal microscope is shown in Figure 13. FCM technique can be used also for visualizing features in living cells and tissues. Picture taken with FCM apparatus is presented in Figure 14.

4. Liquid Crystal Defects Analogies – Kibble’s Mechanism

Study of LC defects is also a very interdisciplinary field of research. Analogies to LC defects can be found in magnetic and condensed matter models, as well as in models of the early Universe [5]. The common point for all this models is their dependence on their symmetry properties. Order parameter in LC samples is easy to control with different parameters like temperature, electric field, while “symmetry dependent” experiments in LC analogous systems are normally very complicated and usually unfeasible. Therefore experiments are performed in LC samples and then their results are transferred into analogous systems by mathematical (topological) rules.

An important analogy to LC defects is the particle physics model of the early Universe evolution, known as Kibble’s mechanism [9]. It proposes several symmetry breaking phase transitions in which defects are supposed to form. At this phase transitions Universe is supposed to break into domains, with the order parameter varying randomly from one domain to another. But this is exactly what happens in nematic LC in “quench” isotropic to nematic phase transition.

When a nematic LC is rapidly cooled (quenched) from the isotropic to nematic phase, nematic order does not form immediately [6]. Instead locally ordered nematic regions of different random orientations grow with time as competition occurs for the final director orientation in the equilibrium nematic phase. Schematic picture of “quench” isotropic to nematic phase transition is shown in Figure 15.

![Figure 15](image.png)

Figure 15: “Quench” isotropic to nematic phase transition: (a) isotropic phase – full symmetry, (b) formation of domains – partly broken symmetry, (c) nematic phase – broken symmetry
This equilibration process is an example of a more general statistical mechanics problem, the growth of order through formation and further on coarsening of domains, when quenched from symmetric state to state with broken symmetry. The interaction equilibration along domains’ walls forms a network of topological defects [6]. Approaching the equilibrium some of these defects annihilate, while some can stay stable. It is clear now, that “quench” isotropic to nematic LC phase transition and phase transitions in evolution of early Universe proposed by Kibble are complete analogues.

But not all types of defects seen in liquid crystals can be used in modelling of early Universe. Some types, e.g. wall defects, point defects, contradict basic observational facts that we know about our Universe, e.g. expansion. On the other hand line defects and strings could be the »seeds« that led to the formation of the »large-scale structure« (e.g. galaxies) we observe today, as well as the anisotropies in the cosmic microwave background. A picture of cosmic microwave background radiation (CMBR) intensity taken with COBE telescope is presented in Figure 16.

![Figure 16: Picture of CMBR intensity taken with COBE telescope. Strong anisotropy can be seen.](image)

We should mention that beside CMBR intensity also other CMB analogues with LC and LC defects exist. The most “famous” is the CMB polarization map, where the polarization map is modelled as rod-shaped molecules laid on a two-dimensional sphere, the sky [11]. In the CMB polarization same defects and similar interaction exist, as in nematic molecules oriented along a sphere with planar boundary condition.

5. Conclusion

LC defects are formed due to boundary conditions on surrounding surfaces or, as presented in section 4, by quenching LC samples from isotropic to nematic phase. Only disclination line and point LC defects are stable, if no external field is present. Typically defects are described by Frank’s elastic model, with introduction of core constants. Two main techniques for experimental study of defects are presented.

Dynamic effects are not treated in this seminar due to their complexity. Typical dynamic processes are annihilation of defects with opposite strength, rearrangement of stable
defects in patterns with well defined spacing between them, wall defects, interaction between defects, etc. These studies are of particular interest because, on one hand, nematic LC are one of the simplest systems with broken symmetry, while on the other hand their properties are general and can be applied in many other branches of physics or other natural sciences.

Applications of LC defects are typically closely connected with the general use of LC. Defects are of particular importance in LC displays and other optical shutters, where LC samples without defects are demanded. Special preparation of surface is therefore needed. A more “direct” application of LC defects is as optical amplifiers by the study of surfaces. From the texture of defects in LC sample shape of boundary surface can be determined. This method can be used for study of biological systems, e.q. molecular membranes of cells from different human tissues [12].

6. Sources