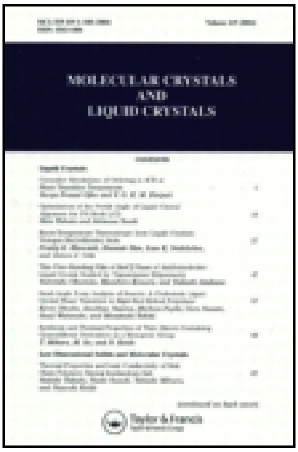

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Visualization of Nematic Director Field With the RGB Color System

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The two-dimensional presentation of the three-dimensional nematic liquid crystal structure can be visualized in various ways: by oriented rotational ellipsoids, bricks, cylinders, or sticks, representing either individual molecules or nematic director field. Here, we give a different approach: the three axes of Cartesian coordinate system are assigned with three colors (red for x*-axis, green for* y*-axis and blue for* z*-axis). We use the proportional mixing of these colors for various directions of the nematic director. Using this technique, different structures of nematic liquid crystals can be visualized clearly, particularly when combined with representation of nematic director field with sticks.*

Keywords nematic liquid crystals; visualization; nematic director; RGB system

1. Introduction

In many branches of natural sciences in education, such as physics topics, the three-dimensional (3D) spatial imagination is crucial for proper understanding of natural phenomena, for instance in the theory of chaos and non-linear dynamics [1–3]. Another example is various kinds of vector fields: electric, magnetic, velocity field in the stream of fluid, etc. Since the presentation of 3D objects is viewed on two-dimensional (2D) screens, it is important for students to gain the ability of correct interpretation of 2D presentation of real 3D objects.

Liquid crystals (LCs) are materials capable of forming liquid crystal phases [4]. They exhibit several extraordinary properties that make them indispensable in our life. They (i) are typical representatives of soft materials, (ii) are relatively easily available, (iii) exhibit a rich variety of different phases and structures, (iv) are transparent and optically anisotropic for

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the visible light to mention just a few of them [5, 6]. Note that their "soft" character makes them very responsive to relatively weak perturbations, so they are important for efficient transport of information in biological systems, or in applications such as LC displays [7]. The response of such soft matter systems to different kinds of weak perturbations has been recently exploited in the investigation of stochastic resonance [8].

Various LC phases may contain different kinds of topological defects, where some translational or orientational ordering is not uniquely defined [9–20]. Defects strongly influence the visual appearance of LCs and they also play important role in various material properties (e.g. plasticity) and in phase transitions. The physics of defects also exhibits several universalities which link to some extent the physics of liquid crystals with other branches of physics, even with particle physics and cosmology [5, 6, 21, 22]. For example, coarsening dynamics of a dense tangle of defects following a sudden phase transition in LCs, where a continuous symmetry is broken, is well described with the general Kibble-Zurek mechanism [23, 24]. This mechanism was originally developed to explain topological defects in cosmologic structures and their role in the early universe. Note also that the group theoretical approaches [21] developed by mathematicians found excellent testing ground in defects realized in LC phases.

The nematic director field can be represented in different ways, one of them being representation with sticks [4]. Rotational ellipsoids are often used to represent individual LC molecules and different colors can be useful to illustrate their directions in 3D space more plastically [25]. Alternatively, bricks with three different edge lengths are suitable to show the orientational ordering of essentially biaxial molecules [26].

In this paper we focus on the simplest case of nematic LCs (NLCs), which exhibit orientational ordering but possess no positional order. The proper visualization of nematic 3D structure is of great importance, particularly for complex structures (such as domains and defects) resulting from competitive ordering factors. We present a means of 3D visualization of nematic director field by red-green-blue (RGB) color system and compare it with commonly known representation with sticks.

2. RGB and Stick Visualization of NLC Structures

We shall briefly call the representation of nematic director field in 3D space by red-green-blue (RGB) color system and commonly known representation with sticks the *RGB* and *stick visualization*, respectively (or *combined visualization* if both types are superposed). Nematic director $\boldsymbol{n}$ is a unit vector corresponding to the local average direction of several NLC molecules. The head-to-tail invariance of nematic director is assumed: $\boldsymbol{n} \equiv -\boldsymbol{n}$. This is the reason why sticks are used to represent nematic director rather than arrows.

We propose the RGB visualization in the following manner. The three perpendicular axes (directions) of Cartesian coordinate system are assigned with three RGB colors (red for x-axis, green for y-axis and blue for z-axis). When the local nematic director has one of these directions, the point is given the corresponding color at that position. For other directions the proportional mixing of the three RGB colors is used. Let us denote the proportions for mixing colors by R, G and B for red, green and blue, respectively, and let the nematic director have the Cartesian components $\boldsymbol{n} = (n_x, n_y, n_z)$. We take the following mixture of colors: $R = n_x^2$, $G = n_y^2$, $B = n_z^2$. We stress that we have no attempt to color the objects representing the director field or individual molecules (such as sticks or ellipsoids), but we color the space points instead since we try to mimic the continuity and smoothness of nematic director field. In this paper, we illustrate five well-known cases of NLC structures in cylinder or sphere with radius normalized to unity.

2.1 Line Defect m = 1/2

The line defect is characterized by the winding number m, which can have integer or half-integer values, either positive or negative [4, 27]. We take thee z–axis as the defect line, where the component n_z is zero and the components n_y and n_y depend only on coordinates x and y, but not on z. We ignore the melting of the nematic order in the defect core and so will be done for the following structures with defects. The winding number m tells how many full angles 2π the nematic director is rotated for when the core of the defect is encircled once. In our case with $m = 1/2$ we can write:

$$\vec{n} = \left(\cos\frac{\varphi}{2}, \sin\frac{\varphi}{2}, 0\right) \tag{1}$$

where $\varphi = \arctan\frac{y}{x}$ is the azimuthal angle. In RGB visualization there is no blue in the color mix (Fig. 1a). The weakness of RGB visualization is that it is not sensitive to the sign of individual components. For example, the locations with $(n_x, n_y, 0)$ and $(-n_x, n_y, 0)$ have the same color, but are clearly distinguished in stick visualization.

2.2 Escaped Radial Structure

This structure is characteristic for NLC confined to long cylindrical cavity where strong homeotropic surface anchoring is applied to the system. The nematic director is perpendicular to the surface at cylinder boundary. Cylindrical confinement of NLC can be achieved, for instance, by Anopore or Nuclepore membranes or capillary tubes [28–32]. To avoid the $m = 1$ line defect at cylindrical axis, which costs a lot of excess free energy the nematic phase is typically either melted near cylindrical axis (z-axis), or the nematic director is escaped in z-direction, depending on various parameters [31, 32]. Here we consider the latter possibility–the so called escaped radial (ER) structure. We shall not go into exact form of ER structure, but we give for pedagogic purpose a simplified formula for nematic director:

$$\vec{n} = (\sin\Omega\cos\varphi, \sin\Omega\sin\varphi, \cos\Omega) \tag{2}$$

where similarly as in Eq. (1), $\varphi = \arctan\frac{y}{x}$, and Ω is the angle between z-axis and local nematic director. Our simplification is in taking the linear dependence of Ω on the distance $\rho = \sqrt{x^2 + y^2}$ of the point from z-axis: $\Omega(\rho) = \frac{\pi}{2} \cdot \rho$. In RGB visualization, points at cylinder boundary have a mixture of red and green colors, while more and more blue color is added on approaching the z-axis (see Figs 1b and 1c for top and side view).

2.3 Double Twisted Structure

This is also a defect-less structure characteristic for chiral NLC with cylindrical confinement. We suppose a strong planar surface anchoring with the easy axis in the azimuthal direction: that is, the nematic director at cylinder boundary is perpendicular both to radial direction and z-axis. On z-axis the nematic director points in z-direction, as in the case of ER structure. The term double twisted (DT) structure indicates that in contrast to commonly known helical (cholesteric) structure of chiral nematics with a single twist axis [4],

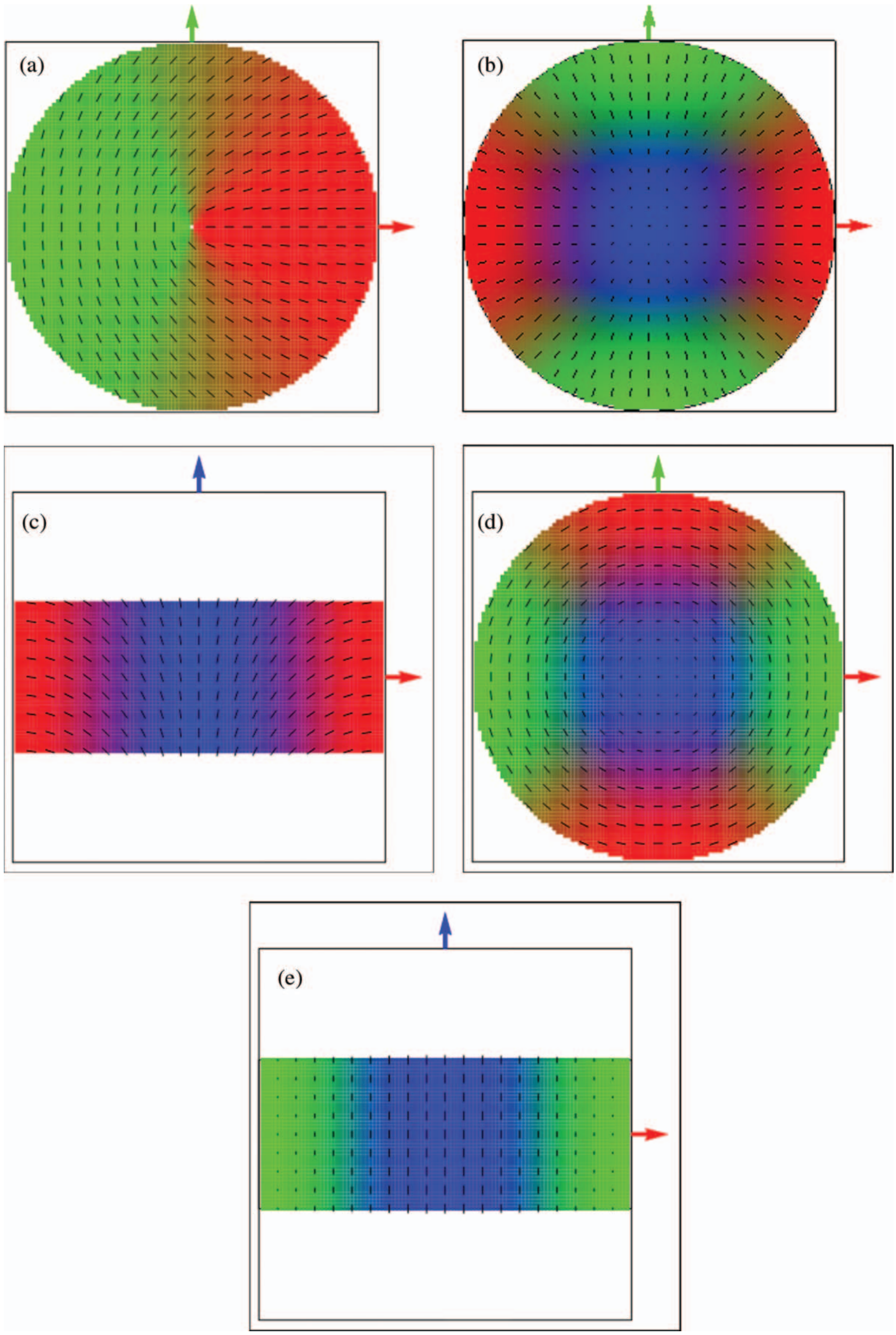

Figure 1. Combined visualization of three cylindrical NLC structures: a) $m = 1/2$ line defect, b) ER structure (top view), c) ER structure (side view, *xz* plane), d) DT structure (top view), e) DT structure (side view, *xz* plane).

there are two perpendicular twist axes for DT structure: in our case x- and y-axes. More concisely, the nematic director is continuously twisted about every local radial axis (and it remains everywhere perpendicular to this axis) what is suggested by theoretical models and confirmed by experiments for some geometries [33–35]. The DT structure is theoretically treated also as the base for some blue phases [33, 36]. Extensive numerical calculations have shown that twist angle does not deviate significantly from the linear dependence on the distance of the point from z-axis [34, 35]. So we can set the model analogous to that of the ER structure:

$$\vec{n} = (-\sin\Omega\sin\varphi, \sin\Omega\cos\varphi, \cos\Omega) \tag{3}$$

with the same meaning of angles φ and Ω as in (2), and $\Omega(\rho) = \frac{\pi}{2}\cdot\rho$ again, where $\rho = \sqrt{x^2+y^2}$. If we compare the corresponding RGB visualization with that of ER structure, we see that the role of blue color is the same, but the red and green colors change their roles (see Figs 1d and 1e for top and side view). For strong nematic chirality or large cylinder radius there may be several turns of nematic director between cylinder axis and its boundary [34, 35]; here we choose the total twist angle just 90° for easier comparison of ER and DB structures.

2.4 Hedgehog Structure

This is a spherically symmetric structure confined to spherical cavity, with a point defect in the center of the sphere. It is forced by strong homeotropic surface anchoring. Spherical or nearly spherical droplets with submicrometer size can be obtained in polymer dispersed liquid crystals [37–41]. The radially oriented nematic director of the hedgehog (HH) structure can be written in the simple form:

$$\vec{n} = \left(\frac{x}{r}, \frac{y}{r}, \frac{z}{r}\right) \tag{4}$$

where $r = \sqrt{x^2+y^2+z^2}$. The corresponding RGB representation is seen in Fig. 2a (just top view of xy plane).

2.5 Bipolar Structure

The bipolar (BP) structure in spherical cavity has two point defects at the two opposite poles on the sphere surface. It is forced by strong planar surface anchoring. If the z-axis is taken as the symmetry axis and the sphere radius is normalized to unity, the poles are at the points $(0, 0, \pm 1)$. The nematic director on the surface of the hole is oriented along the meridians between the poles. Inside the sphere, the nematic director tends to orient more in the z-axis direction when the z-axis is approached. As in the case of ER and DT structures in cylindrical geometry, there were several numerical investigations of the exact bipolar structure. Here again, we take the simplest possible form of nematic director field that describes this structure qualitatively correctly:

$$\vec{n} = \left(-\frac{xz}{\sqrt{1-z^2}}, -\frac{yz}{\sqrt{1-z^2}}, n_z\right) \tag{5}$$

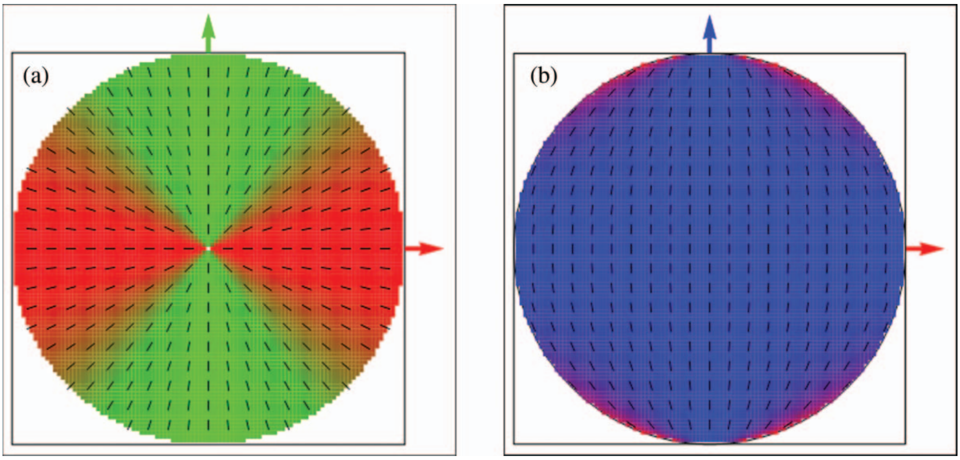

Figure 2. Combined visualization of two spherical NLC structures: a) HH (top view, *xy* plane), b) BP structure (side view, *xz* plane).

where the third component is obtained from normalization condition: $n_z = \sqrt{1 - n_x^2 - n_y^2}$. The corresponding RGB representation is seen in Fig. 2b (just side view - *xz* plane.).

Although just a few main planes (cross-sections of five structures) are presented in Figs. 1 and 2, we have prepared several cross-sections and joined them into animations so that the observer has the feeling of traveling through the whole structure.

3. Visualization Tests with Students

In order to get some feeling about the true comprehension of different types of 3D visualization of NLC structures, we performed a short preliminary test on a small group of physics students (first year course), which were unfamiliar with LCs. Frontal PowerPoint presentation of the five structures was given to students. Before the presentation of the five structures a very brief explanation of the meaning of nematic director as well as stick and RGB visualization was given to students. Next, each structure was presented by a short animation where the structure was scanned through its profile in specific direction. This means, for instance, that when the hedgehog structure was scanned in the top view, planes parallel to *xy* plane (coordinate z varying from -1 to $+1$ with the typical step 0.05) were shown one after another in animation. We used combined visualization (RGB + sticks) in this preliminary test. Immediately after the animation of individual structure the students answered a few questions about the corresponding structure. They had no possibility to review the structure again. Actually, we decided to present the simplest hedgehog structure first and it was used just for initial warm-up: the students received the right answers together with short argumentation of them in order to get a feeling how to deal with the remaining four structures (BP, line defect, ET, DT). There were 25 questions for these remaining structures. The success was roughly half correct answers from all. We also recorded the appropriate time for answering each question (the questions have different levels of difficulty, so they demand different times). On average, about 1 to 2 minutes per question is sufficient. Here is an example of the question in regard to BP structure:

Where is the defect of nematic director (choose the right answer)?

A) In the centre of the sphere.
B) At two locations on the sphere's surface.
C) Everywhere on the sphere's surface.
D) Nowhere at all.

We also received some useful remarks from students after the test. For instance, at least in dynamic animations the combination of colors and sticks seemed very illuminating to them. Next, for each question the animation should be repeated, and consequently the question with the choice of answers should be stated again (animation should be refreshed in memory each time!).

According to this experience, we plan to perform extensive tests for quantization of results. A larger number of students of various study programs will be divided into three subgroups, and for each group one of the three competitive visualizations will be tested. All students' groups will have the same introductory explanation and will answer the same questions; only the type of animation will be different (with RGB colors, sticks or combined).

4. Conclusion

Combination of red-green-blue (RGB) color visualization with the presentation using sticks superposed on RGB background may be very useful to ease the comprehension of complex three-dimensional liquid crystal structures. It could be also used for other vector fields, e.g., for presentation of electric field of dipole: while the direction of the local electric field is illustrated by the RGB color and the stick, its magnitude could be presented by the brightness of the color. The same approach (decreasing brightness) can be used to visualize the drop of the nematic scalar order parameter in the core of the defect.

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