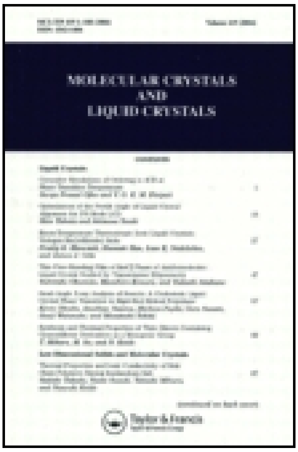

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Disclination Line in θ-Cell as an Indicator of Liquid Crystal Chirality

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We report a new method for the detection and measurement of the chirality of liquid crystal compounds. The method is based on the determination of an azimuth of a disclination line in a θ-cell, with the director aligning unidirectionally at one side and circularly at another one. Experimental observation of disclination rotation was performed with a composition of ZLI-4801-0000 liquid crystal and dopants of opposite-sign chirality (R-2011, S-2011, 7-dehydrocholesterol). Dynamic behavior of the disclinaton line was revealed under the influence of continuous illumination by actinic UV radiation.

Keywords Chirality; disclination; photo-induced transformations; UV irradiation; θ-cell

Introduction

Liquid crystal (LC) devices attract continuously growing interest owing to their ability of optical transformations. Due to high inherent birefringence of LC molecules, oriented (ordered) micrometer-thick LC films are able to modulate efficiently the phase and polarization of a propagating light wave [1,2].

Widely used nematic LCs are characterized with the local averaged anisotropic molecules orientation, called the director, in the plane of a cell (planar orientation), i.e., parallel to the cell walls. In general cases, the planar LC director alignment on one face of a cell can differ from the alignment on another one. To satisfy the boundary conditions, the director has to reorient gradually its azimuth angle, thus producing a twist. The artificially twisted nematic LC resembles a cholesteric one possessing inherent twist structure characterized by a pitch Λ [3]. Twisted nematic LC cells have been widely employed in transmissive and reflective displays [4], and combined twisted LC cells made from reference and tested surfaces are used extensively in studies on the LCs photoalignment properties of various materials [5,6].

The object of our consideration is the LC cell, with parallel to the x-axis rubbing of a front face and circular rubbing of a rear face, designed by Stalder and Schadt [7,8]. The LC cell of this type is called the θ-cell. The origination of the disclination-type defect in the LC orientation and the polarization conflict, which appears due to the rotation of a linear polarization in the twisted LC structure, were analyzed in a recent report [9]. The goal of the present paper is to show a simple method for the detection and measurement of the

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chirality of LC compounds by determination of the azimuth orientation of a disclination line in an LC θ-cell.

θ-Cell Characteristics

Figure 1 schematically gives a picture of LC molecules' orientation along the depth of the cell. The boundary conditions on the cell walls align the director parallel to the x-axis at one side and orient it circularly at another one. Starting from the orientation parallel to the x-axis, the director then rotates to satisfy finally the alignment angle determined by the circular rubbing of the rear substrate. The molecules located along the y-axis do not experience any twist. Generally, the possible twist angles in this configuration do not exceed the values $\pm\pi/2$ with respect to the angle θ_{min}, which minimizes the elastic twist energy. As seen in Fig. 1, the director makes clockwise rotation at the quadrants $x > 0$, $y > 0$ and $x < 0$, $y < 0$, and counter-clockwise rotation at the quadrants $x > 0$, $y < 0$ and $x < 0$, $y > 0$. Along the x-axis ($y = 0$), the twist angle becomes undetermined and a topological defect in the form of a disclination appears. The presence of the defect (disclination line) has been predicted to occur in a θ-cell [7,8] and demonstrated experimentally [9]. With an achiral nematic LC filling the θ-cell, the disclination is oriented parallel to the unidirectional rubbing.

As follows, for achiral nematic LC in a θ-cell, the minimum of elastic energy evidently corresponds to zero twist, i.e., $\theta_{min} = \pi/2$ or $-\pi/2$ in the laboratory reference frame (Fig. 1). However, an addition of some amount of a chiral dopant to the nematic LC will change θ_{min} to $\theta_{min} = \delta \pm \pi/2$, where the angle δ indicates the inner minimum-energy twist angle of the LC composition. According to the expectation, the elastic forces' balance on the maximum-energy angle amounts consequently to $\theta_{max} = \theta_{min} \pm \pi/2$. This conclusion is the main point for further consideration.

To avoid uncertainty with possible one full or multiple pitches within the cell, we assume that the chirality is relatively small ($|\delta| < \pi/2$). While there is not a simple method to visualize the minimum-energy twist angle, it is rather easy to detect the maximum-energy angle θ_{max}, because a disclination line appears along it. The disclination line is

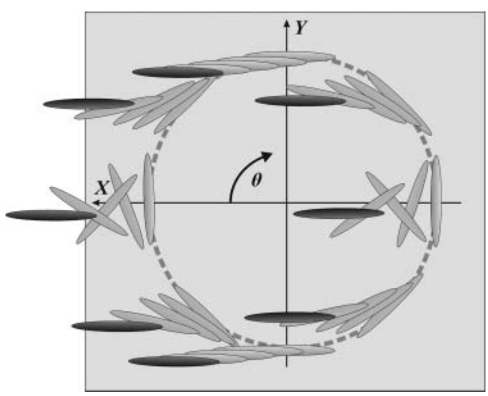

Figure 1. Schematic representation of the nematic LC molecules orientation in the θ-cell. The rear substrate with the circular rubbing (dashed circle) is shown in gray color. The origin of the x, y axes is placed at the center of the circular alignment. The molecules are shown as dark ellipsoids at the front substrate, and light ones in the depth of the cell. The twist angle $\pm\pi/2$ becomes undetermined along the x-axis and a topological defect (disclination) appears.

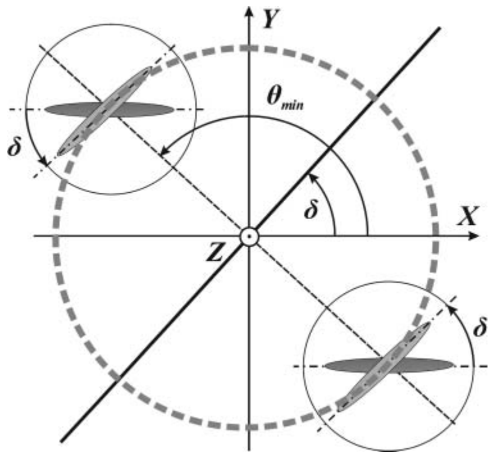

Figure 2. Geometrical sketch of the LC director twist in the θ-cell in the case of certain chirality of the LC. The z-axis is directed toward the observer. The minimum-energy twist configuration is shown in the circles, with the twist angle δ indication. Dark ellipsoids stand for the molecules oriented parallel to the x-axis at the input surface, light ones are oriented along the gray dashed circle at the output surface. Disclination is shown as a solid thick line, the azimuth of the minimum-energy orientation by a dashed line. This configuration corresponds to the right inner minimum-energy twist and δ is positive.

therefore oriented at the angle $\theta_{\max} = \delta \pm \pi$ with respect to the unidirectional rubbing axis. Measuring the azimuth of the disclination gives exactly the inner minimum-energy twist angle δ, as Fig. 2 shows. With the knowledge of the cell thickness d, the pitch Λ can be then calculated as

$$\Lambda = \frac{2\pi d}{\delta}. \tag{1}$$

For instance, the particular value $\delta = \pi/2$ will produce the step from zero twist to one half-pitch (180° twist) along the azimuth $\theta = \pm\pi/2$. According to Equation (1), one-quarter of the pitch minimizes the energy of the LC compound in the cell. In the geometry of Fig. 2, the right-handed chirality of the dopant results in the counter-clockwise rotation of the disclination line.

Materials and Methods

The cell was made from two 1-mm-thick glass substrates covered (spin-coated) with a Kapton polyimide film. The rubbing was produced mechanically, unidirectional for one substrate and using a rotating disk for another one. The used spacers provided a cell thickness of 20 μm. The cell transversal dimensions were 1–3 cm. After filling the cell with the LC compound, we inspected the prepared cells in a microscope. While the originated disclination becomes visible even by eye due to light scattering, the microscope picture makes the measurement of the azimuth angle better. The thickness of the disclination line amounts to 1–1.5 μm. To get the best resolution, the cell was illuminated with the use of an aperture. Illuminating white light was linearly polarized, with the polarization orientation along the unidirectional rubbing at the input surface of the cell. In this geometry, output polarization becomes azimuthal [7–9], which was checked with an analyzer.

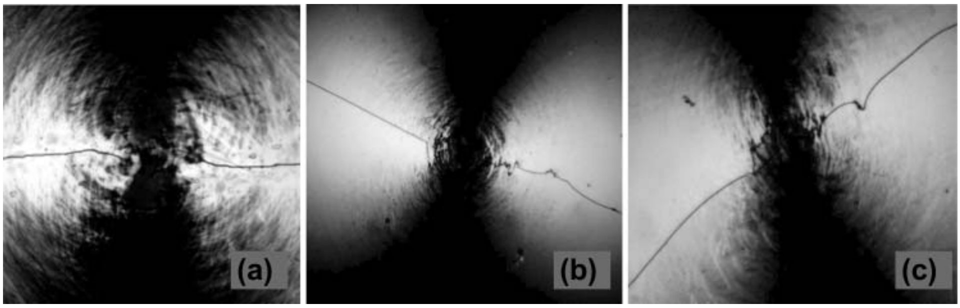

Figure 3. Microscope view of a θ-cell in polarized light: (a) filled with pure nematic 5CB, (b) filled with composition 5CB and R-2011, (c) filled with composition 5CB and S-2011. The width of the windows is 1 mm.

The first used LC was a pure nematic 5CB (4-pentyl-4′-cyano-biphenyl) LC. Figure 3(a) shows the observed picture, with the cell placed between the crossed polarizer and the analyzer. The intensity distribution in this case has a shape according to the Malus law:

$$I(\theta) \propto \cos^2 \theta, \qquad (2)$$

and the disclination line is seen on the bright background. The orientation of the disclination is mainly parallel to the unidirectional rubbing, as expected. The cell impurities, caused by the circular rubbing, distort the picture quality.

Then, the θ-cell was filled with a composition containing right and left-handed chiral dopants, to confirm the effect of the disclination reorientation caused by an LC chirality. We used R-2011 (right-rotating) and S-2011 (left-rotating) chiral dopants (Merck). The concentration of the chiral dopant chosen in both cases was equal or less than 0.5% in order to make the disclination line rotate on a small angle (not exceeding 90°). With the use of the chiral dopants, we definitely detected the unique dependence of the disclination rotation direction on the sign of the dopant chirality, as seen in Figs 3 (b) and (c). To observe the dark line on a bright background, the analyzer was rotated correspondingly. With the right-rotating R-2011 dopant (Fig. 3(b)), the disclination experienced clockwise rotation, with some fluctuations caused by imperfections during the cell manufacturing. In turn, left-rotating S-2011 dopant-induced counter clockwise rotation of the disclination (Fig. 3(c)). Evidently, the method permits easy recognition of the sign of the chirality of a dopant.

To verify the quantitative influence of the chiral properties of the LC compound on the disclination line azimuth, we prepared a solution that contained ZLI-4801-0000 liquid crystal (Merck) and some amount of the chiral dopant 7-Dehydrocholesterol (7-DHC) (Fluka). Figure 4 gives examples of the pictures seen in a microscope without a polarization analyzer. The disclination is detectable as a narrow dark line. There is a break in the continuous disclination at the center due to the mechanical circular rubbing, letting the central zone undefined in the sense of the LC alignment.

With pure achiral nematic ZLI-4801-0000 liquid crystal, the tilt of the disclination is absent and the dark line is horizontal. The addition of 0.17% 7-DHC makes the tilt of the disclination line evident with respect to the horizontal axis (Fig. 4(b)). The direction of the rotation indicates a right twist induced by the dopant. For comparison, Fig. 4(c) gives similar picture for the 0.4% mixture. The orientation of the cells was the same as before (Fig. 3).

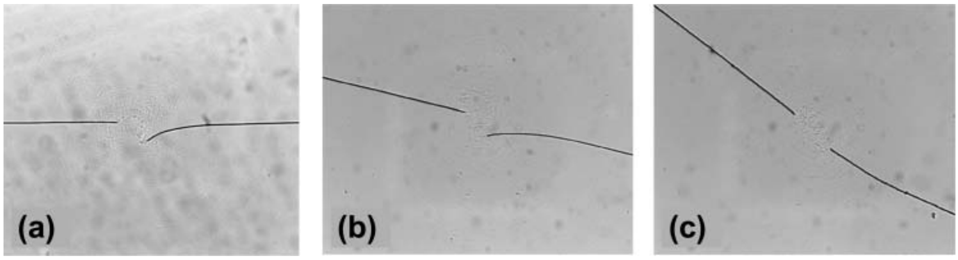

Figure 4. Microscope views of a θ-cell filled with ZLI-4801-0000 liquid crystal and its compositions with the chiral dopant. (a) The disclination line is not tilted with respect to the linear (horizontal) rubbing direction, pure nematic LC. (b) Similar picture for the cell filled with a 0.17% 7-DHC mixture. (c) The same for a 0.4% 7-DHC mixture. The width of the windows shown is 1 mm.

Figure 5 gives the concentration dependence as a summary of the measurement of the disclination azimuth. Within the accuracy of the experiment, the nonlinear proportionality is detected, which is caused probably by a limited solubility of 7-DHC in the LC ZLI-4801-0000 matrix.

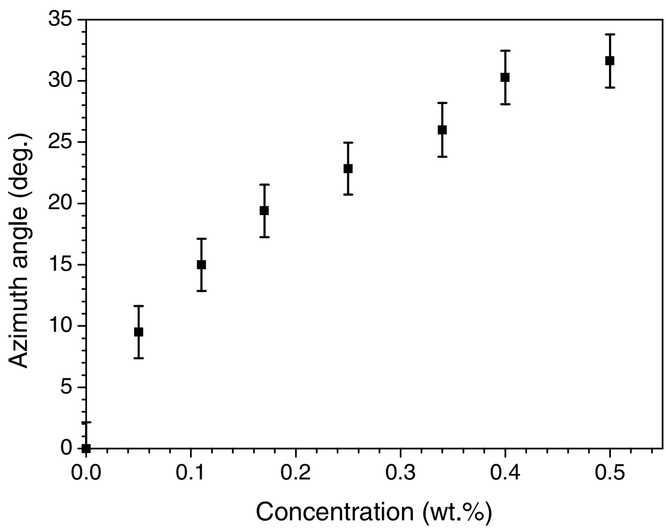

Figure 5. The experimental dependence of the measured azimuth angle of the disclination line versus concentration of the 7-DHC chiral dopant.

Dynamic Variation in the Disclination Azimuth Under UV Illumination

It is known that under the illumination of UV (ultraviolet) radiation in the spectral range 250–350 nm, the chirality of the 7-DHC molecules changes owing to the photo-induced isomerizations (hexadiene ring-opening and further *cis–trans* isomerization) initiated by the UV irradiation [10]. The ability of the chiral dopant to twist a nematic LC results in the continuous rotation of the disclination around the center of the circular rubbing. These real-time variations in the LC compound chirality can be easily visualized with the use of a θ-cell. In this set of experiments, the cell was prepared with one quartz substrate transparent

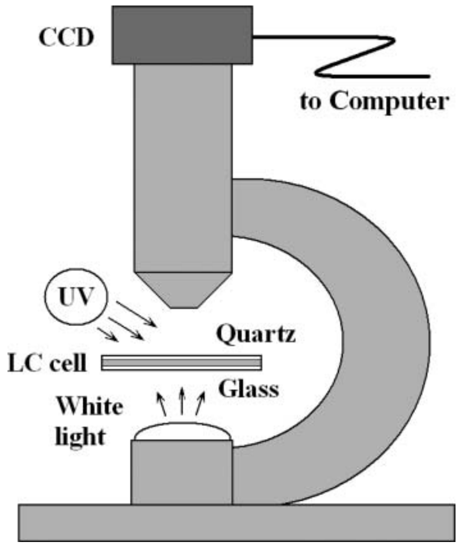

Figure 6. Experimental configuration: the LC cell placed on the microscope stage is illuminated by UV radiation from the mercury lamp. The UV radiation enters the cell through the transparent quartz substrate. White light illuminates the cell from bottom. Images taken with the CCD (charge-coupled device) camera are sent to the computer.

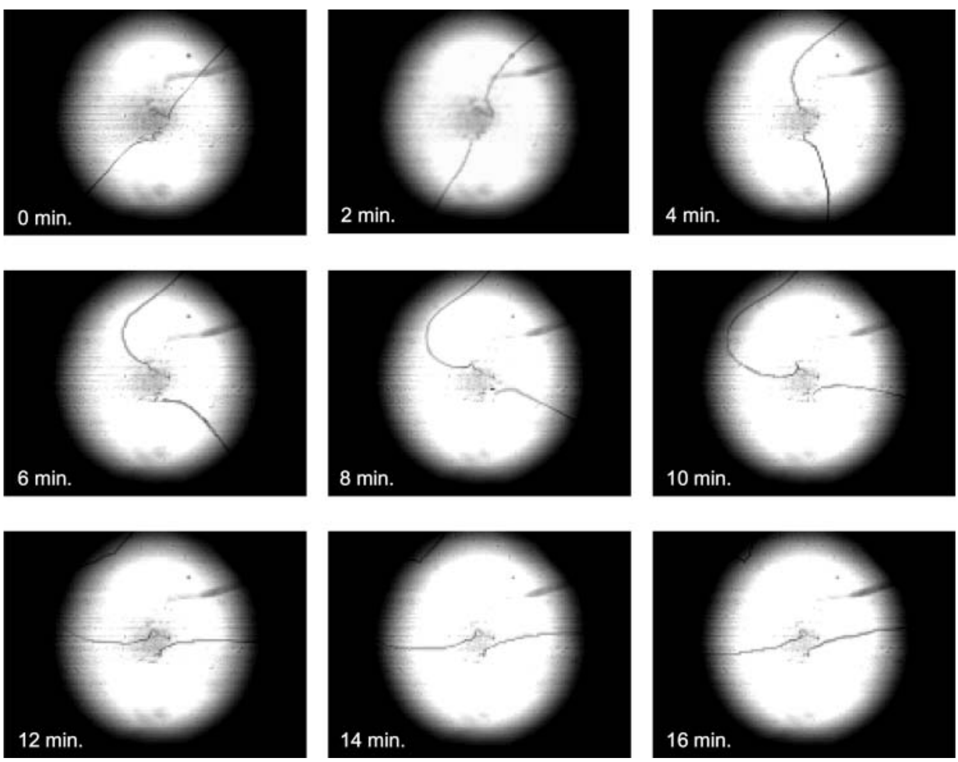

Figure 7. Microscope pictures of the disclination orientation taken in different moments of time, as indicated.

to actinic UV radiation. The quartz surface was covered by polydimethylsiloxane (PDMS) polymer and linearly rubbed. The other substrate was a Kapton polyimide-coated glass plate, rubbed circularly. The concentration of the 7-DHC dopant amounted to 0.3 wt.%.

A sketch of the experimental setup is shown in Fig. 6. UV radiation from a mercury lamp enters the LC cell through the quartz substrate. The exposure time amounted to normally about 20 min. Continuous movies were recorded in real time. Images shown in Fig. 7 give momentary views of the disclination orientation. The visible traces of linear rubbing provide a useful reference for azimuth determination. Because the illuminating white light in this experiment comes from the glass wall rubbed circularly, the observed rotation of the disclination occurs counter-clockwise for the growing right chirality of the composition.

We detected some asymmetry in the disclination line rotation, which is probably caused by nonuniform UV illumination intensity and an influence of the interaction of the LC with the oriented surface, owing to pretilt of the molecules.

Conclusions

The result of this study is the development of a new method for the investigation of LC properties, namely the chirality of an LC compound containing a chiral dopant. The use of a θ-cell permits the detection of the orientation of a disclination line that divides the areas with opposite sign of the twist.

The method permits easy determination of the sign of a dopant chirality due to the unique dependence of the rotation direction of a disclination line on the sign of the dopant chirality. Hence, it complements the known practice of determining the cholesteric screw sense by the Grandjean–Cano method [11], using a wedge-like LC cell placed on a polarization microscope stage, and observing the direction of interference stripes motion with the rotation of the analyzer.

Finally, we demonstrate (at least qualitatively) the ability to observe in real time the dynamic processes of photo-induced transformations of photoliable molecules, accompanied with the variationin their helical twisting power under the influence of actinic UV radiation. This property is of practical importance in view of quantitative measuring of the biologically active UV dose.

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