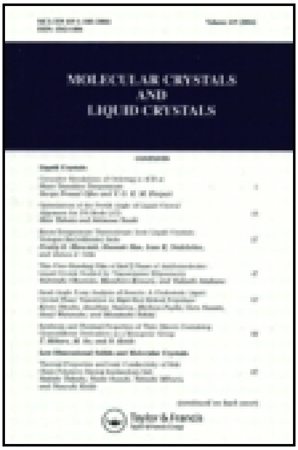

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Director Configurations within Nematic Droplets Doped by Lecithin

O. O. Prischepa [a] , A. V. Shabanov [a] & V. Ya. Zyryanov [a]
[a] L.V. Kirensky Institute of Physics, Akademgorodok, Krasnoyarsk, Russia

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Director Configurations within Nematic Droplets Doped by Lecithin

O. O. Prischepa
A. V. Shabanov
V. Ya. Zyryanov
L.V. Kirensky Institute of Physics, Akademgorodok,
Krasnoyarsk, Russia

The series of polymer dispersed liquid crystals films based on polyvinylbutyral-nematic 5CB composition doped by lecithin have been prepared. The characteristic textures of nematic droplets with various concentration of surfactant have been investigated and their orientational structures have been identified. It allowed to reveal the novel director configurations which are transient between bipolar and radial structures. Using the computational method to minimize elastic energy of director field distortions in the droplet bulk and applying the inhomogeneous boundary conditions, the orientational structures have been obtained and these are analogous to the observed ones.

Keywords: director configurations; polymer dispersed liquid crystal; surfactant

INTRODUCTION

Polymer dispersed liquid crystal (PDLC) films are intensively studied in recent years because of their application in electro-optical devices. The optical characteristics of PDLC light shutter strongly depend on the nematic director configuration imposed by droplet wall. Mostly in PDLC films the bipolar structure with two point surface defects (boojums) occurs upon tangential anchoring and the radial structure with a point defect (hedgehog) in the droplet center upon perpendicular (homeotropic) anchoring. These structures were observed first by Lehmann [1] and investigated in detail later in [2–4].

Volovik and Lavrentovich [5] considered a possible transformation of director configurations inside nematic droplets with gradually

Address correspondence to O. O. Prischepa, L.V. Kirensky Institute of Physics, Akademgorodok, Krasnoyarsk 660036, Russia. E-mail: p_oksana@iph.krasn.ru

changed surface anchoring from tangential to homeotropic and predicted two scenarios of the modification. One of them was realized in their experiment with the composition of glycerol and nematic droplets doped by lecithin and accompanied with the appearance of additional disclinations. In this case a gradual change of boundary conditions was provided with variation of temperature in the range of nematic phase. Another scenario without the formation of any additional defects has been found in [6] for set of PDLC films based on polyvinylbutyral (PVB) and nematic 5CB doped by lecithin with varying content. In this work we study in more detail for the last case the director configurations that are transient between bipolar and radial ones and simulate the orientational structures of such nematic droplets and their corresponding textures.

EXPERIMENT

The 4-n-pentyl-4′-cyanobiphenyl (5CB) nematic liquid crystal was chosen for the study. Transition temperatures $\langle$crystal $\leftarrow$ (22°C) $\rightarrow$ nematic $\leftarrow$ (35°C) $\rightarrow$ isotropic liquid$\rangle$. At $T = 22^{\circ}C$ and $\lambda = 0.589\,\mu m$ the refractive indices of 5CB are $n_{\parallel} = 1.725$ and $n_{\perp} = 1.534$ [7]. PVB was used as a polymer matrix. This polymer is transparent in the visible region and provides tangential anchoring with the molecules of mesomorphic alkylcyanobiphenyl derivatives [8]. The refractive index of PVB is $n_p = 1.492$ at $T_c = 22^{\circ}C$ and $\lambda = 0.589\,\mu m$.

As in [6] the gradual change of boundary conditions at polymer-nematic interface is produced by the variation of lecithin admixture. In the LC droplets with lecithin impurity the long axes of surfactant molecules are arranged perpendicular to the surface so that their polar groups are attached to the interface, while the nonpolar fragments (flexible alkyl chains) are directed toward the bulk of the LC (see Fig. 1) [8].

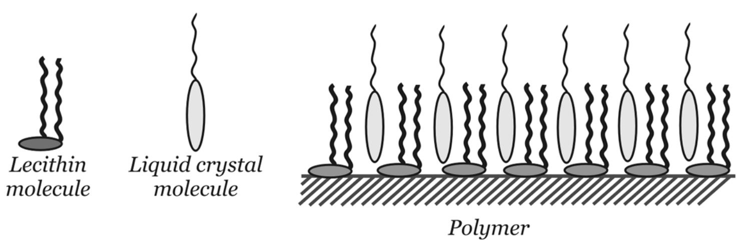

FIGURE 1 The schematic representation of the arrangement of lecithin and LC molecules at the interface.

Due to such structural ordering the lecithin molecules provide the homeotropic orientation of LC molecules at the interface. The samples of PDLC film have been prepared by SIPS (solvent induced phase separation) method with the use of ethyl alcohol as a common solvent for all used components. Content of LC is 55%, the PVB and lecithin concentrations varied within $41.5 \div 45.0$ and $0 \div 3.5$ wt%, respectively. Adjusting the rate of solvent evaporation it is possible to vary the size of droplets and morphology of PDLC film. The LC droplets formed a monolayer with a size dispersion of $4 \div 16$ μm. The study of droplet textures in obtained PDLC films we carried out by using a polarizing microscope both in geometry of crossed polarizers and in the linearly polarized light with an analyzer switched-off.

In PDLC films under study the director configuration within droplets greatly depends on the lecithin concentration (see Fig. 2). In nematic droplets without surfactant the only typical bipolar configuration realizes. The addition of surfactant more 0.1% leads to the appearance of the droplets having the radial structure and the structure with a single surface defect. The more the lecithin's content the more number of droplets with the new structures. When surfactant content is more 1.6% the droplets with bipolar configuration disappear. Under 3.5% lecithin concentration we observed the radial configuration only in the whole of nematic droplets.

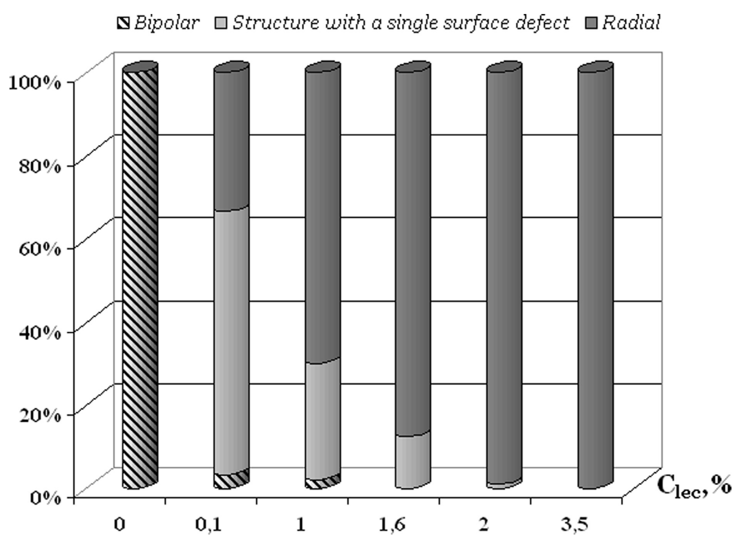

FIGURE 2 Diagram of relative content of NLC droplets with the different director configurations in PDLC films depending on concentration of lecithin.

As it has been shown earlier [2–5], the perfect *bipolar configuration* is characterized with two point surface defects or so-called ⟨boojums⟩ on the opposite sides of droplets (see Fig. 3a and Fig. 4a). In the crossed polarizers two symmetrically arranged hyperbola-shaped extinction bands are seen (Fig. 3a, central column) these emanate from the droplet poles and gradually expand. When observing with a single polarizer the point surface defects are especially distinctly visible as dark dots (Fig. 3a, right column). Intense local light scattering

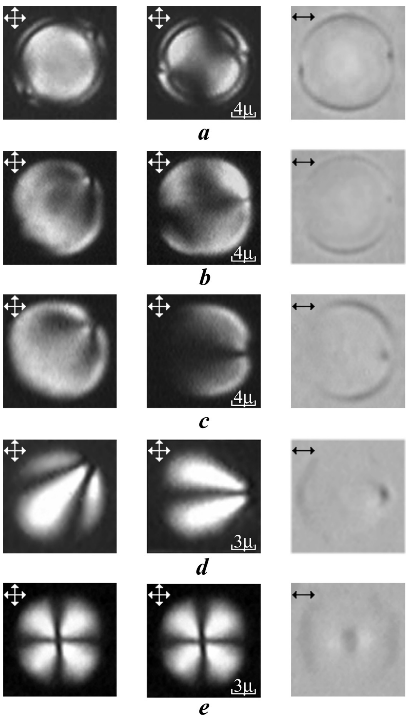

FIGURE 3 Textures of nematic droplets of 5CB dispersed in PVB with different lecithin content C_{lec}. (left column) Microphotographs in the geometry of crossed polarizers (shown by white arrows) with droplet symmetry axis directed at $\alpha = 45^\circ$ to the polarizer. (central column) Microphotographs in the geometry of crossed polarizers with symmetry axis directed at the angle $\alpha = 11^\circ$ (***a***, ***b***) and $\alpha = 0^\circ$ (***c***, ***d***) to the polarizer. (right column) Microphotographs in the linearly polarized light with relative orientation of the polarizer (shown by black arrows) and symmetry axis as in central column. (***a***) Bipolar droplet, $C_{lec} = 0\%$; (***b***) droplet with a destructed left boojum, $C_{lec} = 0.08\%$; (***c***) monopolar droplet, $C_{lec} = 0.1\%$; (***d***) droplet with the surface hedgehog structure, $C_{lec} = 2.0\%$; (***e***) droplet with the radial structure, $C_{lec} = 2.6\%$.

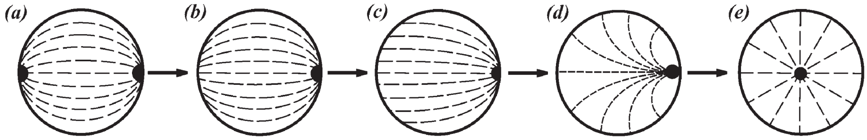

FIGURE 4 The sequence of schematic director configurations in nematic droplets with different lecithin concentration which results from analysis of the above shown textures. The arrows are directed toward the increase of the surfactant content. (***a***) bipolar droplet; (***b***) droplet with a one destructed boojum; (***c***) monopolar structure; (***d***) surface hedgehog structure; (***e***) radial structure.

of any polarization is caused with a sharp optical inhomogeneity near the defects. Similarly, the sections of droplet boundaries where a light polarization coincides with the local director orientation are well visible as dark lines due to the large gradient of refractive index $n_{ll} - n_p$ is realized here. On the contrary, the boundary sections with the orthogonal arrangement of director and light polarization are seen least distinctly as the gradient of refractive index $n_\perp - n_p$ is minimal in this area.

The structures with a single surface defect should be identified carefully. Detailed observations using polarizing microscope show that these structures may be very different, in spite of the fact that their textural patterns have similar features. At lecithin 0.08% content one of the boojums in bipolar droplets destructs (see Fig. 3b). This is clearly seen in left region of texture in Figure 3b (right column) in the geometry with a single polarizer. The extinction band near the decaying boojum does not converge but expands (Fig. 3b, central column). In the remaining region of the droplets the textural pattern is similar to the bipolar structure. It should be noted that in this case the boundary conditions are inhomogeneous. The director field distribution in such droplet can be represented by the configuration shown in Figure 4b. When moving from destructed defect along the surface to the remaining point defect the director anchoring changes gradually from the homeotropic state to a tilted one and finally becomes tangential.

The director lines become straighter (Fig. 4c) if the lecithin concentration in samples increases up to 0.1%. The region of homeotropic and tilted director orientations rises so that the structure can be named *monopolar* (Fig. 3c). In the crossed polarizers when a symmetry axis of droplet coincides with one of them, a single extinction band is seen in the droplet. It emanates from the right point defect, strongly expands and fills almost the entire left half of the droplet. The texture of the droplet's right half remains analogous to the bipolar structure.

In the samples with the lecithin content equal to 2.0% the droplets with *the surface hedgehog structures* (Fig. 3d and Fig. 4d) predominate. In such droplets in crossed polarizers three extinction bands are observed (Fig. 3d, central column) when their symmetry axis is parallel to a polarizer. The central band goes along the symmetry axis but it is narrower in comparison with one in the monopolar structure (Fig. 3c). Two side bands emanate from the point defect at the approximate angle 50° to the symmetry axis on each side of it. As a result the droplets with the surface hedgehog structures look like cones in this geometry although they have in fact a round form (Fig. 3d, left and right columns). From the consideration of the corresponding director configuration shown in Fig. 4d one can understand the origin of the three above-mentioned extinction bands.

As it is shown in Figure 2 the droplets with *the radial structure* startforming already at small addition of the lecithin and their number in the PDLC film increases while the surfactant concentration rises. This configuration is well-known. It is characterized with a single point defect in the centre of droplets (see Fig. 3e and Fig. 4e), so-called ⟨radial hedgehog⟩ [2–5]. When observing in geometry of crossed polarizers four dark bands are seen in the shape of the Maltese cross (Fig. 3e, left and central columns. Turning of PDLC sample at any angle does not change their orientation (see Fig. 3e).

CALCULATION OF THE DIRECTOR CONFIGURATIONS

The structures described above (Fig. 4a–e) we calculated within the three-dimensional model by means of minimization of the orientation part of free energy

$$F = \frac{1}{2}\int K\Big[(\nabla \cdot \mathbf{n})^2 + (\nabla \times \mathbf{n})^2\Big]dV \qquad (1)$$

of the LC volume using the method developed in [9,10]. Here, K is an elastic constant, **n** is a nematic director. The problem was solved in one-constant approximation with the elastic modulus $K = (K_{11} + K_{22} + K_{33})/3$. The K_{ii} values were taken from [11]. The minimum of F in Eq. (1) was found by the variational method in Cartesian coordinate system and applying the boundary conditions correspondent to the experimentally observed ones.

Our simulation have showed that the bipolar (radial) configuration (Fig. 5a, e) is realized for the rigid tangential (homeotropic) anchoring, respectively, at the whole droplet boundary that is in agreement with [12]. To obtain the transient structures (Fig. 4b–d) we used inhomogeneous boundary conditions. For example, in order to calculate the

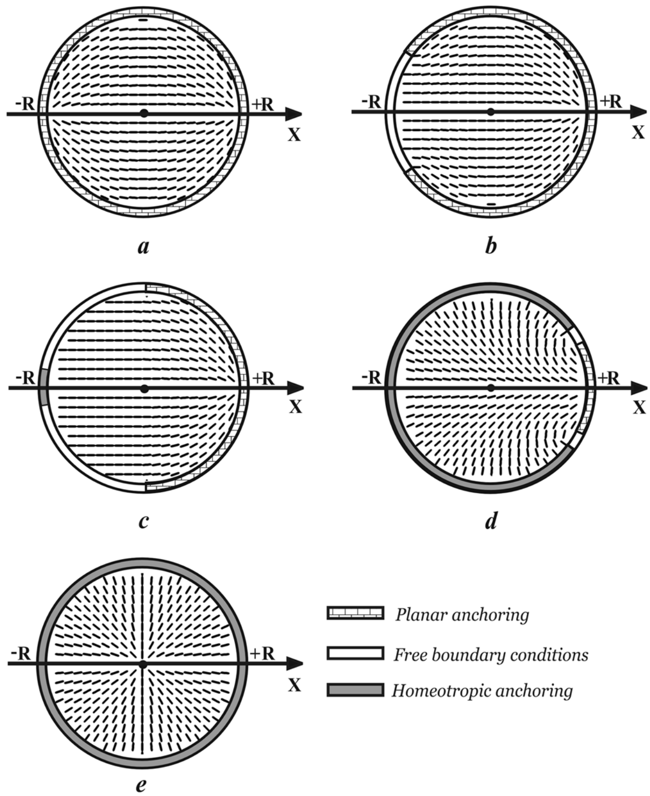

FIGURE 5 The director configurations in the diametrical cross section coinciding with a symmetry axis of spherical nematic droplets obtained by theoretical calculation using inhomogeneous boundary conditions. (***a***) Bipolar structure; (***b***) droplet with a one destructed boojum; (***c***) monopolar structure; (***d***) droplet with the configuration to be similar to surface hedgehog structure; (***e***) radial structure.

structure with one destructed boojum the rigid tangential anchoring have been assigned for all surface points whose X coordinates are within the interval $-0.8\,R \leq X \leq +R$ (Fig. 5b). On the rest of the surface with the coordinates $-R \leq X < -0.8\,R$ the boundary conditions were free. The resulting director configuration shown on Figure 5b is similar to the configuration presented in Figure 4b. It should be noted that the minimization procedure results in the tilt director orientation at the free boundary which gradually changes from homeotropic (tilt angle $\theta = 0^\circ$ at point $X = -R$) to tangential ($\theta = 90^\circ$ at $X = -0.8\,R$).

Further, we have carried out the calculation of monopolar structure (Fig. 4c), where the tangential anchoring was applied to the region $0 \leq X \leq +R$. The boundary conditions within interval $-0.98\,R < X < 0$ were free and within $-0.02R \leq X \leq -0.98\,R$ were homeotropic (Fig. 5c). To calculate the director field distribution for the droplet with the surface hedgehog structure we used the following parameters. Homeotropic orientation is in limit $-R \leq X \leq +0.84\,R$ and the region of rigid tangential anchoring is $+0.92\,R \leq X \leq +R$. The rest of the boundary is free (Fig. 5d). The obtained director configuration is not a perfect surface hedgehog structure shown in Figure 4d but it is a closer analog to it which can be obtained in framework of simulation model used.

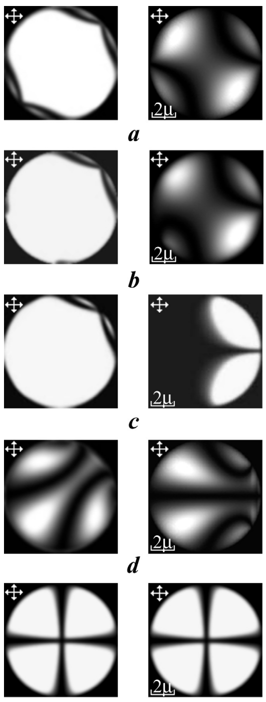

FIGURE 6 Theoretically calculated textures of spherical nematic droplets in the geometry of crossed polarizers for the director configurations shown in Figure 5. (left column) Textures for angle $\alpha = 45^\circ$ between droplet symmetry axis and polarizer. (right column) Textures for angle $\alpha = 11^\circ$ (***a***, ***b***), and $\alpha = 0^\circ$ (***c***, ***d***) between droplet symmetry axis and polarizer. (***a***) Bipolar structure; (***b***) droplet with a destructed left boojum; (***c***) monopolar structure; (***d***) droplet with the configuration to be similar to surface hedgehog structure; (***e***) radial structure.

The data was used to simulate the correspondent textural patterns in the geometry of crossed polarizers by applying the theoretical approach described in [13]. One can see (Fig. 6) that the textures calculated for the same droplet size and angle α agree mainly with the microphotographs in Figure 3.

CONCLUSION

Thus, the textural patterns and corresponding director configurations of nematic droplets doped by various amount of lecithin and dispersed in polymer have been described. A set of orientation structures intermediate between the bipolar and radial configurations have been revealed. They can exist simultaneously in the same sample that may be resulted from the inhomogeneous distribution of surfactant in PDLC film.

The data obtained prove that upon changing boundary conditions from tangential to homeotropic the gradual transformation of the bipolar structure into a radial one may occur through a sequence of equilibrium director configurations without the formation of additional disclinations, as it was predicted previously by topological analysis in [5].

The use of inhomogeneous anchoring which is appropriate for real boundary conditions enables to obtain the director configurations and textural patterns of nematic droplets to be analogous to the experimentally observed ones. Some discrepancies between experiment and simulation data which are especially visible in Figure 3d and Figure 6d can be explained by imperfection of the used theoretical model which needs improving in future. For example, the boundary conditions used in the simulation should be correspond more exactly to real ones, namely it is necessary not only to determine the boundary areas with $\theta = 0^\circ$ and $\theta = 90^\circ$ and to take into account an actual distribution of director tilt angle on rest of droplet surface.

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