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THE R- AND H- DEFECTS IN A CYLINDRICAL CAPILLARY

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Abstract Having based on well-known limiting cases, we constructed the approximate solutions of equilibrium equations for nematic liquid crystals for the radial (R) and hyperbolic (H) point defects in a capillary with normal boundary conditions. On the contrary to the point of view accepted before we have to claim that because of equivalence of both directions of "escaping" along the capillary axis the bound R- and H-defects occurred instead of non-singular disclination. The comparative analysis of elastic fields of free and bound R- and H-defects has been given. It has been shown that the boundaries do not influence on topology of the elastic fields and far from the singularities the structure coincides with the structure of a non-singular disclination. It has been obtained that the difference between the energies of the R- and H-defects in the bound state is half as much as the correspondent value for the free defects.

INTRODUCTION

Within the continuum theory approximation the equilibrium deformed state of liquid crystal is described by the closed system of differential equations for the director field $\vec{n}(\vec{r})$. Analysis of these equations allowed one to establish the possibility of existence of a great variety of structural defects,[1] which are the singularities of director fields, and many of them were discovered experimentally.[2] A considerable body of work is devoted to the study of free defects in boundless media not to be under influence of external forces.[3,4] It is common knowledge however, that external forces, among which are those dependent on the presence of boundary surfaces, cause the equilibrium elastic field to change essentially and in consequence can control processes of defect creation and conditions of their stability.[5]

The objective of our work is to study the structure of defects that arise when the planar disclination of strength $k = +1$ $\left(L_{+1}^{(p)}\right)$[1)] escapes into the third dimension in a cylindrical capillary filled nematics under normal boundary conditions. The consideration is symplified by using one constant approximation of the elastic theory of partially ordered media.[6]

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[1] From this point onward, the symbol ( ) will be used to mark the defects bound by the cylinder surface.

APPROXIMATE FUNCTIONS

To achieve the objective let us assume director components as follows

$$n_1 = \sin\alpha\cos\beta,\ n_2 = \sin\alpha\sin\beta,\ n_3 = \cos\alpha, \tag{1}$$

where α and β are polar and azimuth angles of local coordinate system that define the direction of vector $\vec{n}(\vec{r})$ at a given point and must obey the equilibrium equations[1]

$$\begin{aligned} &\nabla^2\alpha - \sin\alpha\cos\alpha(\nabla\beta)^2 = 0, \\ &\nabla^2\beta + 2\cot\alpha(\nabla\alpha, \nabla\beta) = 0. \end{aligned} \tag{2}$$

If, according to[5], we assume that the escaping of planar disclination takes place along the only one direction of capillary axis Oz (one-sided instability) then $L_{+1}^{(p)}$ transforms into non-singular disclination $L^{(ns)}$, which is described in cylindrical coordinates by the following solutions of Equations (2)

$$\alpha_{I\infty}(\rho) = 2\tan^{-1}\left(\frac{\rho_0}{\rho}\right)^I,\ I = \pm 1,\ \alpha_{+\infty} = \pi - \alpha_{-\infty} \ \text{ and } \ \beta(\varphi) = \varphi. \tag{3}$$

Here ρ_0 is a capillary radius exceeding the critical value at which the process $L_{+1}^{(p)} \to L^{(ns)}$ becomes energetically preferable,[5] parameter I indicates the "escaping" along positive (I = +1) or negative (I = -1) directions of the cylinder axis. This solution provides the nor-mal conditions at the boundary surface ($\alpha(\rho_0) = \pi/2$) and "escaping" along Oz ($\alpha(0) = 0, \pi$).

The one-sided instability of disclination $L_{+1}^{(p)}$ does not bring to a creation of singularities in a cylinder and breaks the symmetry of "escaping". When we assume that both directions of axis Oz are equivalent, two-sided instability will arise, the planar point defect of radial type arising within symmetry plane xy. In this case angular function β is unchanged, but function α (3) becomes to be dependent on coordinate z as well. Then system (2) can be reduced to the following equation

$$\frac{\partial^2\alpha}{\partial z^2} + \frac{\partial^2\alpha}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial\alpha}{\partial\rho} - \frac{\sin\alpha\cos\alpha}{\rho^2} = 0. \tag{4}$$

The particular solutions of Equation (4) are functions

$$\alpha^R = 2arctg\left\{\frac{\sqrt{\rho^2+z^2}-z}{\sqrt{\rho^2+z^2}+z}\right\}^{1/2},\ \ \alpha^H = \pi - \alpha^R, \tag{5}$$

that describes free R- and H-defects.

The attempts to obtain an exact analytical solution of Equation (4) under the boundary and "escaping" conditions mentioned above haven been unsuccessful so far. However knowledge of analytical functional relations offers some advantages over the solutions obtained by computation. So it seems appropriate to try to find an approximate function $\alpha^{(i)} = \alpha^{(i)}(\rho,z)$ that satisfies to all the physical conditions of the problem and the limiting cases, namely:

1. As $L_{+1}^{(p)}$ escapes, director lines are unchanged and form the planar R-defect within symmetry plane xy

$$\alpha^{(i)}(\rho,z \to \pm 0) = \pi/2, \qquad (i = R,H).$$

2. The influence of a core of the point defect onto the structure of its elastic field is negligibly small far away from xy-plane

$$\alpha^{(R)}(\rho, z \to \pm\infty) = \alpha_{\mp\infty}, \quad \alpha^{(H)}(\rho, z \to \pm\infty) = \alpha_{\pm\infty}.$$

3. Director is perpendicular to the capillary surface

$$\alpha^{(i)}(\rho \to \rho_0, z) = \pi/2, \; \beta = \varphi.$$

4. There are not any singularities on the symmetry axis of the cylinder, except when $z = 0$

$$\alpha^{(i)}(\rho \to 0, z \neq 0) = 0, \pi.$$

5. As the radius of the capillary ρ_0 is increased, the point defect arisen from the two-sided instability of disclination $L_{+1}^{(p)}$ transforms into corresponding free defect

$$\alpha^{(i)}(\rho_0 \to \infty, \rho, z) = \alpha^{i}(\rho,z).$$

Functions $\alpha^{(i)}$ that satisfy to the above-listed criteria can be represented as follows

$$\alpha^{(R)} = 2arctg\left\{\frac{\sqrt{\rho^2 + z^2 q_+^2} - zq_-}{\sqrt{\rho^2 + z^2 q_+^2} + zq_-}\right\}^{1/2}, \quad \alpha^{(H)} = \pi - \alpha^{(R)}, \text{ where } q_\pm = 1 \pm \frac{\rho^2}{\rho_0^2}. \quad (6)$$

Now on substituting Equation (6) into (4), we get that the greatest deviation of the left side of Equation (4) from zero is reached in a small vicinity of points $|z| = 0.26\rho_0$, $\rho = 0.71\rho_0$, its maximal value being 0.39. At any other points the left side of Equation (4) is little different from zero.

THE STRUCTURE OF THE (R)- AND (H)-DEFECTS

Now let us consider the structure of elastic fields that are described by functions $\alpha^{(i)}$, $\beta = \varphi$. Substituting director components (1) into the differential equations for director lines and taking into account Equation (6) we shall obtain the following

$$\varphi = \text{const and } \pm q_- \frac{d\rho}{\rho} = D\frac{dz}{z}, \text{ where } D^2 = 1 + \frac{4z^2}{\rho_0^2}. \tag{7}$$

The solution of Equation (7) is the implicit function

$$C + \left[\ln\frac{\rho}{\rho_0} - \frac{1}{2}\left(\frac{\rho}{\rho_0}\right)^2 \right] = \pm\left(D + \frac{1}{2}\ln\frac{D-1}{D+1} \right). \tag{8}$$

Figure 1 represents director lines designed according to formula (8). It is shown that the signs "±" define fields of bound (R)- (Figure 1a) and (H)- (Figure 1b) defects respectively. Despite distortions under the influence of the boundary surfaces these fields are topologically equivalent to those of the corresponding free defects and at large values of z coincide with the field of non-singular disclination $L^{(ns)}$.[5]

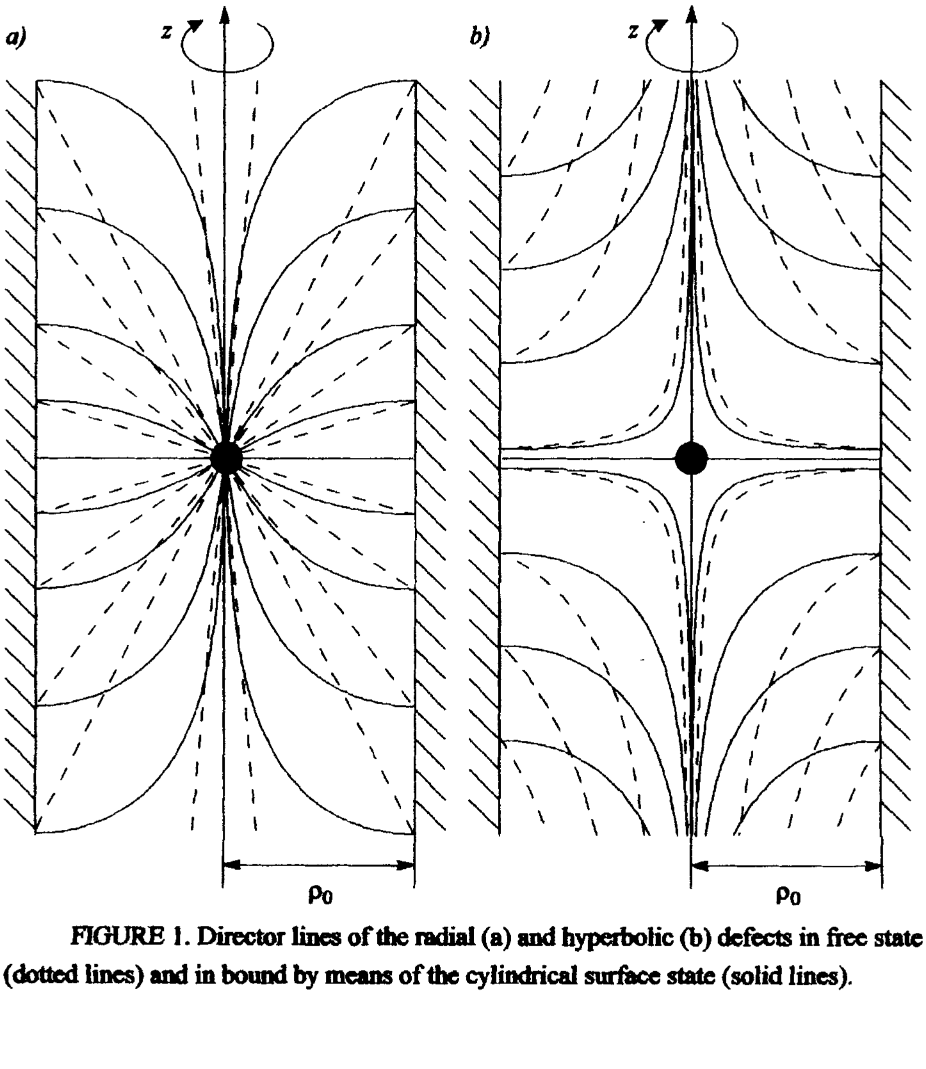

FIGURE 1. Director lines of the radial (a) and hyperbolic (b) defects in free state (dotted lines) and in bound by means of the cylindrical surface state (solid lines).

THE ELASTIC ENERGY

Of special interest is to study the influence of the boundary surface on the energies of point defects in a cylindrical capillary and to compare them with the corresponding energies of free defects. In this paper we shall restrict our consideration to the analysis of the energy gap between (R)- and (H)-defects.

The energy of elastic deformations can be defined by the following formula[1]

$$E = \frac{K}{2}\int_V \left\{(\nabla\alpha)^2 + \sin^2\alpha(\nabla\beta)^2 + 2\sin\alpha\left(\vec{n}\left[\nabla\alpha, \nabla\beta\right]\right)\right\} dV, \tag{9}$$

where K is a Frank constant and V is a volume of nematics.

Because of the axial symmetry of the system considered the domain of integration is conveniently bounded by a cylinder with radius of base ρ_1 and height $2z_1$, which is coaxial with the cylindrical capillary. Upon integrating Equation (9) with respect to coordinate φ, we represent the energy gap as

$$\Delta_i(\rho_1, z_1) = -2\int_0^{\rho_1} d\rho \int_0^{z_1} \sin^2\alpha \frac{\partial\alpha}{\partial z} dz, \tag{10}$$

where Δ_i are the differences of energies of defects in free state ($i = 1$, $\alpha = \alpha^R$) or in bound one ($i = 2$, $\alpha = \alpha^{(R)}$), which are normalized to $4\pi K$.

On substituting Equation (5) into (10), we obtain for the free defects

$$\Delta_1 = \frac{E^R - E^H}{4\pi K} = 2\int_0^{\rho_1} \rho^3 d\rho \int_0^{z_1} \frac{dz}{\left(\rho^2 + z^2\right)^2} = \rho_1 \operatorname{arctg}\frac{z_1}{\rho_1} + z_1 \ln\left(1 + \frac{\rho_1^2}{z_1^2}\right). \tag{11}$$

Expanding Equation (11) as a power series in $\frac{\rho_1}{z_1}$ until the first non-zero term we get

$$\Delta_1\left(z_1 >> \rho_1\right) = \frac{\rho_1}{2}\left(\pi - \frac{5}{3}\frac{\rho_1^3}{z_1^3}\right). \tag{12}$$

Now let us calculate the energy gap for the bound defects. After substituting Equation (6) into (10), the corresponding transformations Δ_2 can be written as the sum

$$\Delta_2 = \frac{E^{(R)} - E^{(H)}}{4\pi K} = \sum_{i=1}^{3} J_i\left(\rho_1, z_1\right), \tag{13}$$

where $J_1 = \rho_1 u(\rho_1)$, $\quad J_2 = \int_0^{\rho_1} u(\rho)\frac{d\rho}{q_+} = u\left(\frac{\rho_1}{\rho_0}\right)u(\rho_1) + g\left(\rho_1, z_1\right),$

$$J_3 = 8\int_0^{\rho_1} q_-(q_+-1)\rho^2 d\rho \int_0^{z_1} \frac{z^2 dz}{\left(\rho^2+z^2 q_+^2\right)\left\{\sqrt{\rho^2+4z^2(q_+-1)}+\rho\right\}} = \frac{\rho_0}{6}\left(\frac{\rho_0}{z_1}\right)^2\left(1-\frac{6}{\tilde{q}_+}+\frac{9}{\tilde{q}_+^2}-\frac{4}{\tilde{q}_+^3}\right),$$

$$u(\rho) = \mathrm{arctg}\left(\frac{q_+ z_1}{\rho}\right), \quad \tilde{q}_\pm = 1 \pm \frac{\rho_1^2}{\rho_0^2},$$

$$g(\rho_1, z_1) = \frac{\rho_0}{4}\ln\left(D+\sqrt{D^2-1}\right)\left(\ln_- - \ln_+\right) + \left(G_+ - G_-\right),$$

$$\ln_\pm = \ln\left(1+\frac{\rho_1^2}{\rho_0^2}\frac{a_\pm}{a_\mp}\right), \quad G_\pm = \frac{\rho_0}{2}\left\{\pi u\left(\frac{\rho_1}{a_\pm}\right) - a_\pm \int_0^{\rho_0}\frac{\ln\left(1+\rho_1^2/\rho^2\right)}{a_\pm-\rho^2}\right\}, \quad a_\pm = \frac{2z_1}{D\pm 1}.$$

Here integral J_3 has been calculated in the approximation $\frac{\rho_1}{z_1} << 1$ since it vanishes when $\rho_0 \to \infty$ and decreases rapidly as z_1 increases. The value of the energy gap for the bound defects is then defined by the following expression

$$\Delta_2(\rho_1, z_1) = \rho_1\left(\frac{2\rho_0}{\rho_1}u\left(\frac{\rho_1}{\rho_0}\right)-1\right)u(\rho_1) + 2\left(g(\rho_1, z_1) + J_3(\rho_1, z_1)\right). \tag{14}$$

Consider some important limiting cases. To do this we shall take into account the equalities

$$g(\rho_1, z_1) = \begin{cases} \frac{z_1}{2}\ln\left(1+\frac{\rho_1^2}{z_1^2}\right), & \rho_0 \to \infty, \quad (15) \\ \frac{\rho_0^2}{2z_1}\frac{\tilde{q}_+-1}{\tilde{q}_+}\left(2\frac{\rho_0}{\rho_1}u\left(\frac{\rho_1}{\rho_0}\right)-1\right), & z_1 >> \rho_1, \quad (16) \end{cases}$$

that result from the passages corresponding to the limits in integral J_2. Then it follows from Equation (15) that

$$\Delta_2\ (\rho_0 \to \infty) = \Delta_1.$$

This means that the influence of the capillary surface on the defects becomes negligibly small when the surface is infinitely distant and the energy gaps of the free defects and the bound ones are the same.

Taking $\rho_1 = \rho_0$ in Equations (14) and (16), we can write Equation (14) in the approximation $z_1 >> \rho_0$, which is of principal interest

$$\Delta_2\left(z_1 >> \rho_0\right) = \frac{\pi}{2}\rho_0\left(\frac{\pi}{2}-1\right) - \frac{\rho_0}{12}\left(\frac{\rho_0}{z_1}\right)^2. \tag{17}$$

Going to the limit $z_1 \to \infty$ in Equations (17), (12) and also substituting $\rho_1 = \rho_0$ in the latter, we obtain

$$\lim_{z_1 \to \infty} \frac{\Delta_2}{\Delta_1} = 0.571.$$

It follows that the energy gap for the free R- and H-defects is approximately twice as much as for the bound defects.

DISCUSSION AND CONCLUSIONS

The construction of an approximate solution of equilibrium equations (2) on the basis of well-known limiting cases has allowed us to conclude that in a cylindrical capillary instead of non-singular disclination $L^{(ns)}$ point defects arise as a result of symmetrical "escaping" of disclination $L^{(p)}_{+1}$. The visual identification and the analysis of limiting cases $\rho_0 \to \infty$ and $\rho \to 0$, $z \to 0$ have shown that these point defects are singularities of R-type ("node ") and H-type ("saddle"), their structure coinciding with that of non-singular disclination when $z_1 \to \pm\infty$. At $|z_1| >> \rho_0$ director lines of (R)- and (H)-defects are described by the same functions

$$z(\rho) = C_{\pm} \pm \frac{\rho_0}{2} \left\{ \ln \frac{\rho_0}{\rho} - \frac{1}{2} \left(\frac{\rho}{\rho_0} \right)^2 \right\}, \quad C_+ > 0, \; C_- < 0$$

that differ essentially from the asymptotic relations for R- and H-defects in free state.

The distortion of director lines of point defects in a cylinder causes the elastic energy to increase by comparison with their free state. The difference between the values Δ_1 and Δ_2 points out that the cylindrical surface influences the point defects in different ways. In fact, if we accept the value of deviation of an energy level of a free defect when it is placed into an infinitely-long cylinder ($z_1 \to \infty$), that is $\delta_i = E^{(i)} - E^i$, as a measure of the influence of a boundary field on the defect, then the unequality $\delta_H > \delta_R$ follows from the unequality for the width of the energy zones. The latter means that the surface field distorts director lines and increases the elastic energy of the hyperbolic defect considerably more in comparison with those of the radial defect. Moreover, the independence of Δ_i on coordinate z at large distances from a defect core points to the fact that the energies $E^{(i)}$ and E^i can include either the same terms depending on z and having the finite limit at $z_1 \to \infty$ or only non-divergent terms. It can be shown accurately that the latter is true for the energies E^H and E^R with a cylindrical domain of integration. But if calculating the elastic energy we take the spherical domain of radius r, the energies of the R- and H-defects and also the size of the energy gap will be linear functions of r and diverge as r increases.

Thus, under the assumption that both directions of "escaping" along the capillary axis are equivalent, point defects of (R-) or (H)-types with distorted director lines in comparison with the free defects arise as a result of instability of disclination $L_{+1}^{(p)}$ in a cylindrical capillary. The degree of distortion of director lines decreases when a capillary radius increases, and far from the singularity the lines are lines of non-singular disclination $L^{(ns)}$. It seems reasonable to say that it is because of the coincidence of director lines at the asymptotical limit that the width of the energy gap is finite at $z_1 \to \infty$ and defined only by the elastic field in the vicinity of the singularity.

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