



Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics

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ENCAPSULATED LIQUID CRYSTAL ORIENTATION AND OPTICAL PROPERTIES IN A SPHERICAL CAPSULE

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Abstract Both analytical and numerical solutions of LC equilibrium Eqs in a polymeric spherical capsule have been discussed. Experimental evidence supporting theoretical data are presented.

INTRODUCTION

The importance of films obtained by the use of low-molecular liquid crystals (LC) encapsulated in a polymeric matrix has been growing. Long-term stability, large screen creation capability, relaxation properties improvements - all these are major advantages of such materials. When LC is introduced into hydrophobic polymers (polyvinyl alcohol derivatives) spherical capsules are formed¹. We have investigated experimentally and theoretically the LC orientation behaviour within a spherical capsule.

THEORETICAL RESEARCH

To obtain LC orientation arrangement in one spherical bulk the expression free energy density F was used². Omitting the external fields effect this expression is as follows:

$$F = \frac{1}{2} \{ K_1 (\text{div} \vec{n})^2 + K_2 (\vec{n} \cdot \text{rot} \vec{n} + q)^2 + K_3 (\vec{n} \times \text{rot} \vec{n})^2 \} \quad (1)$$

where \vec{n} is the unit vector of the long axes orientation molecule, i.e. director, K_i is the Frank elastic constants, $q = 2\pi/p$, p is an undisturbed ChLC structure helical pitch.

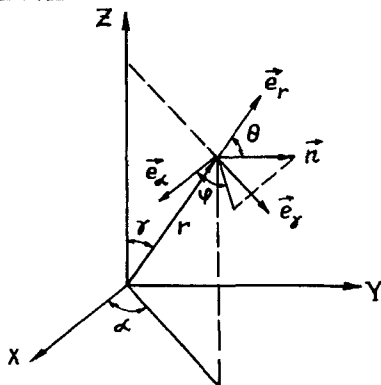


FIGURE 1 Molecular orientation at the capsule surface

Vector \vec{n} in the following geometry (Fig. 1) can be represented as

$$\vec{n} = \vec{e}_z \cos \theta + \vec{e}_y \sin \theta \cos \varphi + \vec{e}_x \sin \theta \sin \varphi, \quad (2)$$

where the angles θ and φ depend on the three spherical coordinates: r , θ , φ .

It is difficult to obtain analytical function of θ and φ on all the three coordinates, hence, a simple approach to the spherically symmetric case was considered. We have also supposed only one radial disclination to be present in the bulk, and the calculation was carried out far away from it. Having made the above allowances and skipping all intermediate operations, we present the eventual LC molecule equilibrium Eqs system in the spherical bulk

$$f_{\theta_{zz}} + \frac{1}{2} \frac{\partial f}{\partial \theta} \theta_z^2 + 2 \frac{1}{r} \theta_z - \frac{1}{2} \frac{\partial g}{\partial \theta} \varphi_z^2 + (K_2 q \cdot \varphi_z + \frac{K_1}{r^2}) \sin 2\theta = 0 \quad (3)$$

$$\frac{1}{r^2} \cdot \frac{d}{dr} [r^2 (q \varphi_r - K_2 q \cdot \sin^2 \Theta)] = 0 ; 0 \leq r \leq R,$$

where R is the sphere radius, and the "r" index denotes differentiation over r .

LC molecule distribution in the bulk is determined by the Eq. (3) and by a present molecular orientation at the LC/polymer interface. The surface orientation is characterised by the angle between the director and the boundary plate as well as by the anchoring energy.

For the geometry adopted this orientation can be planar ($\Theta = \pi/2$), homeotropic ($\Theta = 0$) and oblique ($0 < \Theta < \pi/2$). In addition, cases of "strong anchoring" and those of weak one are distinguished. The analytical solution of the system (3) for a case when ($0 < \Theta < \pi/2$) is cumbersome, therefore a numerical solution was preferred. A particular case of $\Theta = \pi/2$ could be solved analytically. Solutions for both strong and weak anchoring were obtained.

If on the interface LC-polymer tangential orientation is present, $\Theta|_{r=R} = \pi/2$, then in the case of strong anchoring (φ_R is present on the interface)

$$\varphi = q(r - R) + \varphi_R.$$

In the case of weak anchoring ($d\varphi/dr$ are present on the interface)

$$\varphi = q r + \frac{R^2 (q - q_R)}{r}.$$

If the molecule orientation on the interface is arbitrary in the sphere, it is determined as follows:

$$\varphi_z = q + \frac{c}{z^2}, \quad \theta = \pi/2.$$

Thus, if the molecules on the sphere - ChLC interface are oriented tangentially, then depending on the anchoring nature, a cholesteric can torque either with a constant or variable helix pitch. If the tangentiality condition is not realized, a transition layer whose size is of the order of the helix pitch, starts appearing next to the interface (Fig. 2). Hence, spheric capsule formation contributes to the tangentiality

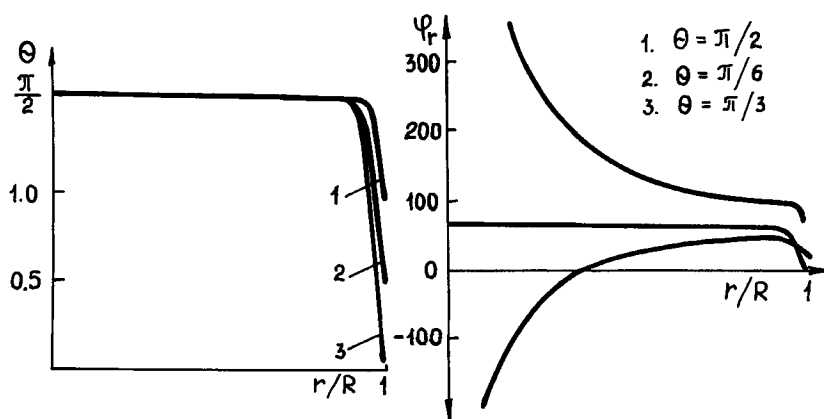


FIGURE 2 Radial dependences of azimuth angle (a) and helical pitch (b) for different boundary conditions

al orientation of the ChLC molecules inside the sphere.

EXPERIMENTAL DATA

To verify the results obtained theoretically, the optical properties of the ChLC polymer system were studied experimentally. The degree of molecules ordering

inside the sphere was evaluated from the spectral parameter of the order³. The calculated spectral order being: for the ChLC planar texture between two plates = 0.92, for the polymer film = 0.75. The high value of the order spectral parameter confirms a close to tangential ChLC orientation in spheric capsules.

Orientational additives (Chromolan) introduced into the film composition lead to deformed transmission peaks. They become broad asymmetric, with the transmission intensity decreasing. These data testify to the weak anchoring of ChLC molecules with the capsule surface and to the presence of a transition layer on the ChLC - polymer interface. The ChLC - polymer anchoring being non-rigid, a change of the orientant nature chemistry may lead to an arbitrary ChLC molecule orientation on the interface, causing in turn the formation of helices of various pitches and, as a consequence, the existence of several selective fields inside the capsule⁴.

Having discussed the ChLC optical properties in a polymer matrix, we came to the conclusion that a ChLC tangential texture characterised by the high selective reflection coefficient was realized in the capsules.

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