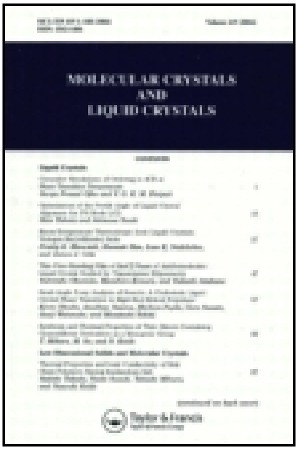

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INFLUENCE OF TRANSVERSE FREDERIKS PERIODIC DEFORMATION ON OPTICAL PHASE SHIFT IN A NEMATIC LIQUID CRYSTAL CELL

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A periodic deformation can arise in a nematic liquid crystal (NLC)-cell with unidirectional planar alignment, when the NLC with positive susceptivity anisotropy is subjected to an external magnetic field. Such a periodic Frederiks distortion occurs, both in the case of strong- and weak-anchoring, if the ratio twist- to splay-elastic constants is lower than a critical value: the cell behaves as a diffraction grating. Here the optical phase retardation of a transmitted polarized light beam normally incident on the sample is studied in the approximation of small distortion, in order to find its dependence on the anchoring conditions. We show that the distortion periodicity goes as the 2nd-harmonic of the in-plane grating, close to Frederiks periodic threshold.

Keywords: diffraction grating; Frederiks transition; Nematic liquid crystals; periodic distortion; phase retardation

1. INTRODUCTION

When the intensity of a magnetic field $\boldsymbol{H}$ normal to the walls of a nematic liquid crystal (NLC) cell with positive susceptivity anisotropy and initial unidirectional planar alignment exceeds a certain threshold H_a, the symmetry with respect to the normal to the cell plates is broken, and the NLC undergoes the well known second order Frederiks transition, which has been described as dependent on one "order" parameter [1], the tilt angle θ (accounted with respect to the cell plates). The angle θ turns out to be dependent only on the co-ordinate z normal to the cell walls.

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Lonberg and Mayer were the first [2] to show that, if the twist distortion definitely costs less energy than the splay, i.e., if the elastic ratio between the twist- and the splay-elastic constants $r = K_{22}/K_{11}$ is less than a critical value r_c, then applying a magnetic field with increasing intensity, at a value $H_p < H_a$ also the azimuth symmetry with respect to the initial planar orientation is broken, and a biperiodic transition takes place. It is driven by two "order" parameters, the twist angle φ and the tilt angle θ, both dependent by the co-ordinate y along the initial in-plane alignment and not only on z. In particular, the twist angle φ and the tilt angle θ are periodic function of (y,z), with definite wave vectors $(q,\ k)$ respectively, thus providing periodic stripes [3,4]. Such stripes were investigated via numerical approach in the same planar geometry and also in the case of inclined alignment of the undisturbed director profile [5,6], and in polymer nematics with large elastic anisotropy [7] and planarly treated surfaces. Thus the periodic pattern driven by an external field define a unidimensional in-plane diffraction grating, modulated along the out-of-plane z direction. This is very interesting from both fundamental- and application point of view, since the diffraction grating appears for $H_p < H < H_a$, is driven by H, and depends not only on the material characteristics but also on the surface treatment, since the surface anchoring affects both thresholds H_p, H_a.

The purpose of the present work is to describe the main feature of the diffraction grating modulated by the external field $\boldsymbol{H}$, predicting the behavior close to the threshold H_p of the phase difference $\Delta\Phi$ of a transmitted light beam with normal incidence with respect to the undeformed director profile in various anchoring- and elastic conditions.

2. THEORY

Let us consider a nematic liquid crystal with positive susceptivity anisotropy and small elastic ratio between the twist- and the splay-elastic constants, filling a planar cell defined by the $[xyz]$ frame of reference (see Fig. 1). The $[xy]$ plane is assumed to be parallel to the cell walls. The cell thickness is D_z, the cell plates being at $z_1 = -D_z/2$ and $z_2 = D_z/2$, respectively. Both plates are properly treated in order to favor the nematic alignment along the x-axis, with the same anchoring strengths at both sides (symmetrical anchoring conditions). If a magnetic field $\boldsymbol{H}$ with sufficient intensity parallel to the z-axis is applied, a biperiodic distortion along $(y,\ z)$-axis can occur. In the frame of the first order continuum theory, the energetic cost of such a distortion can be calculated. The corresponding bulk free energy density is given by [1]:

$$f_{bulk} \equiv \frac{1}{2}\left\{K_{11}s^2 + K_{22}t^2 + K_{33}b^2\right\} - \frac{1}{2}\chi_a(\hat{\mathbf{n}}\cdot\boldsymbol{H})^2, \tag{1}$$

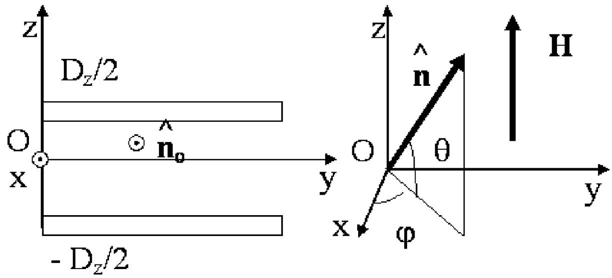

FIGURE 1 Cell scheme with initial unidirectional planar alignment of the NLC-director profile, H = 0; local director n(y, z) periodically distorted in the presence of a magnetic field ***H*** normal to the cell plates above the threshold. The polar angle θ(y, z) is the tilt angle, the azimuth φ(y, z) is the twist angle.

where $\mathbf{s} \equiv \hat{\mathbf{n}}\nabla \cdot \hat{\mathbf{n}}$, $\mathbf{t} \equiv \hat{\mathbf{n}} \cdot curl\,\hat{\mathbf{n}}$, $\mathbf{b} \equiv \hat{\mathbf{n}} \wedge curl\,\hat{\mathbf{n}}$ are the splay vector, the twist pseudo-scalar and the bend vector, respectively, related to the corresponding elastic constants K_{ii}, and χ_a is the magnetic susceptivity anisotropy. The director $\hat{\mathbf{n}}$ can be expressed as $\hat{\mathbf{n}} = \hat{\mathbf{i}}\cos\varphi\cos\theta + \hat{\mathbf{j}}\sin\varphi\cos\theta + \hat{\mathbf{k}}\sin\theta$, being $\varphi = \varphi(y,z)$ and $\theta = \theta(y,z)$. The surface free energy density essentially depends on the anchoring type and following the Rapini-Papoular covariant description [8,9] is:

$$f_{surf} = -\frac{1}{2}W_\varphi\left(\hat{\mathbf{n}}\cdot\hat{\mathbf{i}}\right)^2 + \frac{1}{2}W_\theta\left(\hat{\mathbf{n}}\cdot\hat{\mathbf{k}}\right)^2, \tag{2}$$

where W_θ and W_φ are the anchoring strengths for tilt and for twist, respectively.

Close to the Frederiks periodic threshold $\theta \ll 1rad$, $\varphi \ll 1rad$, so that the problem can be linearized, giving: $s = \theta_z + \varphi_y, t = \theta_y - \varphi_z, b = 0$, where the index means derivative with respect to the mentioned component. Then the total reduced free energy density $g = 2f/K_{11}$ can be written as:

$$g = g_{bulk} + g_{surf} = \left[\left(\theta_z + \varphi_y\right)^2 + r(\theta_y - \varphi_z)^2\right] - h^2\theta^2 + (l_\theta D_z)^{-1}\theta^2 \\ + r(l_\varphi D_z)^{-1}\varphi^2, \tag{3}$$

where $r = K_{22}/K_{11}$ is the elastic ratio between the twist- and the splay-elastic constants, $h^2 = \chi_a H^2/K_{11}$ is the reduced square magnetic field, while $l_\theta = K_{11}/W_\theta\, D_z$, $l_\varphi = K_{11}/W_\theta\, D_z$ are the reduced extrapolation lengths for tilt- and twist, respectively. In the case of strong anchoring, l_θ and $l_\varphi$vanish and $g = g_{bulk}$ only.

The equilibrium state is found when there is a complete balancing of the torques acting on the system both in the bulk and at the surface. The first balancing is described by the Euler–Lagrange equations and the second by the boundary conditions [10].

The Euler–Lagrange equations read:

$$\begin{cases} r\theta_{yy} + \theta_{zz} + (1-r)\varphi_{yz} + h^2\theta = 0, \\ \varphi_{yy} + r\varphi_{zz} + (1-r)\theta_{yz} = 0, \end{cases} \tag{4}$$

where the reduced field $h \equiv H\sqrt{\chi_a/K_{11}}$ is present in the "tilt" equation only, but the two equations are coupled. Since the boundary conditions are symmetrical, it is enough to consider only one surface for instance at $z_1 = -D_z/2$, giving:

$$\begin{cases} \big(\varphi_y(y,z_1) + \theta_z(y,z_1)\big) - (l_\theta D_z)^{-1}\theta(y,z_1) = 0, \\ (\varphi_z(y,z_1) - \theta_y(y,z_1)) - (l_\varphi D_z)^{-1}\varphi(y,z_1) = 0. \end{cases} \tag{5}$$

It has to be noted that the boundary conditions turn out to be explicitly independent of r.

In the case of periodic Frederiks transition, the solutions can be represented by:

$$\begin{cases} \theta = \theta^* \exp[i(pz + qy)] \\ \varphi = \varphi^* \exp[i(pz + qy)] \end{cases} \tag{6}$$

By putting Eqs. (6) into the bulk equations, for a fixed q value four solutions are found: $p = \pm k,\ \pm im$, related through the following relation:

$$p^2 = \frac{h^2}{2} - q^2 \pm \frac{1}{2}\sqrt{h^4 + 4\frac{1-r}{r}q^2h^2}. \tag{7}$$

So the most general solutions read:

$$\begin{cases} \theta = (A\cos kz + B\cosh mz)\cos qy; \\ \varphi = (a\sin kz + b\sinh mz)\sin qy; \end{cases} \tag{8}$$

By substituting these last solutions (8) into the Euler–Lagrange (4), two self-consistency relations are found:

$$\begin{cases} \dfrac{1}{R} \equiv \dfrac{A}{a} = \dfrac{(1-r)kq}{k^2 - rq^2 - h^2} = \dfrac{q^2 + rk^2}{(1-r)kq}, \\ \dfrac{1}{T} \equiv \dfrac{B}{b} = \dfrac{(1-r)mq}{h^2 + m^2 - rq^2} = \dfrac{-q^2 + rm^2}{(1-r)mq}, \end{cases} \tag{9}$$

this means that only two integration constants are independent. Considering the boundary conditions (5) with the solutions (8) and the constraints of Eqs. (9), a system homogeneous in the two integration constants is derived, which has not trivial solutions only if the coefficients determinant vanishes:

$$\det\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = 0. \tag{10}$$

The determinant elements in the case of weak anchoring are:

$$\begin{cases} M_{11} = l_\theta^{-1}\cos[k(h,q,r)D_z/2] + (qR-k)\sin[k(h,q,r)D_z/2]; \\ M_{12} = l_\theta^{-1}\cosh[m(h,q,r)D_z/2] + (qT+m)\sinh[m(h,q,r)D_z/2]; \\ M_{21} = l_\varphi^{-1}R[k(h,q,r);q,r]\sin[k(h,q,r)D_z/2] \\ \qquad + (q+kR)\cos[k(h,q,r)D_z/2]; \\ M_{22} = l_\varphi^{-1}T[m(h,q,r);q,r]\sinh[m(h,q,r)D_z/2] \\ \qquad + (qT+q)\cosh[m(h,q,r)D_z/2]. \end{cases} \tag{11}$$

Equation (10) provides the dispersion relation between q and the external field h: in other words, it can be considered as an implicit definition of the function $h = h(q)$. The minimum value of such a function $h_p = h(q_p)$ is evidently the threshold field for the arising of the periodic Frederiks transition; the corresponding q_p is the initial wave vector of the in-plane periodic distortion close to this reduced threshold h_p.

For each value of h such as $h_p < h < h_a$, the cell behaves as a modulated diffraction grating, with pitch dependent on h. In the approximation of a small amplitude y-distortion ($\theta < 10\,\mathrm{mrad}$), i.e., near the Frederiks periodic threshold, the multiple scattering through the in-plane grating can be neglected. The optical phase retardation of a polarized monochromatic light beam, normally incident on the sample, can be evaluated as follows [11,12]:

$$\Phi(y) = \frac{2\pi}{\lambda}\int_{-D_z/2}^{D_z/2} n_{eff}(\theta(y,z))dz, \tag{12}$$

where λ is the monochromatic light wavelength and the effective refractive index is given by $n_{eff} = n_o\left(1-\rho\cos^2\theta\right)^{-1/2}$, where $\rho \equiv 1-(n_o/n_e)^2$, n_o, n_e being the ordinary, extraordinary indexes, respectively. In Figure 2 the refraction index ellipsoid is shown in both cases of a) undeformed initial alignment and b) local distorted structure with tilt angle θ. In the case of undistorted system, when the h field is below the Frederiks periodic threshold, the phase retardation is given by

$$\Phi_o = \frac{2\pi n_e}{\lambda}D_z. \tag{13}$$

In order to show the influence of the periodic deformation on the phase retardation the phase difference $\Delta\Phi(y) = \Phi(y) - \Phi_o$ will be considered.

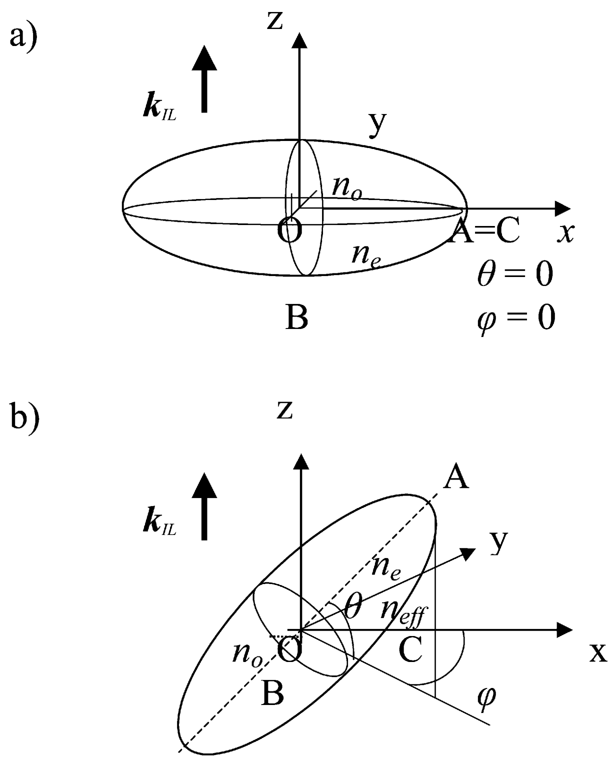

FIGURE 2 Refraction indexes ellipsoid in the case of unidirectional planar alignment along x-axis, a), and in the case of local distorted alignment along OA-axis, b). Reasonable data (assumed from 5CB at room temperature), $n_e = 1.5869$, $n_o = 1.4832$ at wavelength $\lambda = 633$ nm. The incident light wave vector is k_{il}, normal to the cell plates.

Developing at the second order in θ, the optical phase retardation turns out to be:

$$\Delta\Phi(y) \propto \frac{\pi n_e^3}{\lambda n_o^2} \cos^2 qy, \tag{14}$$

being then characterized by the 2nd harmonic of the actual in-plane distortion.

3. NUMERICAL CALCULATION

In the case of strong anchoring the boundary conditions (5) result more simply:

$$\begin{cases} \theta(z = \pm D_z/2) = 0, \\ \varphi(z = \pm D_z/2) = 0, \end{cases} \tag{15}$$

and the dispersion relation coefficients (11) reduce to

$$\begin{cases} M_{11} = \cos[k(h,q,r)D_z/2]; \\ M_{12} = \cosh[m(h,q,r)D_z/2]; \\ M_{21} = R[k(h,q,r);q,r]\sin[k(h,q,r)D_z/2]; \\ M_{22} = T[m(h,q,r);q,r]\sinh[m(h,q,r)D_z/2]. \end{cases} \tag{16}$$

This allows to recover that there exists a critical value of the elastic ratio r, preventing the appearance of the periodic distortion [1–3]. In the case of strong anchoring it is $r_c = 0.303$. If the anchoring is weak, r_c depends on the anchoring strengths. Below such critical value, for any fixed r a periodic solution can be found, determining via minimization of Eq. (10) both the corresponding wave vectors of the periodicity along the y,z-directions (q_p, k_p, m_p) and the threshold value of the magnetic field $h_p(q_p)$. In Figure 3 the corresponding values of q_pD_z, k_pD_z, m_pD_z are shown for different values of r. It is evident that the wave vectors vanish when r is approaching its critical value r_c, as it is by definition expected, since above r_c only an aperiodic deformation is allowed.

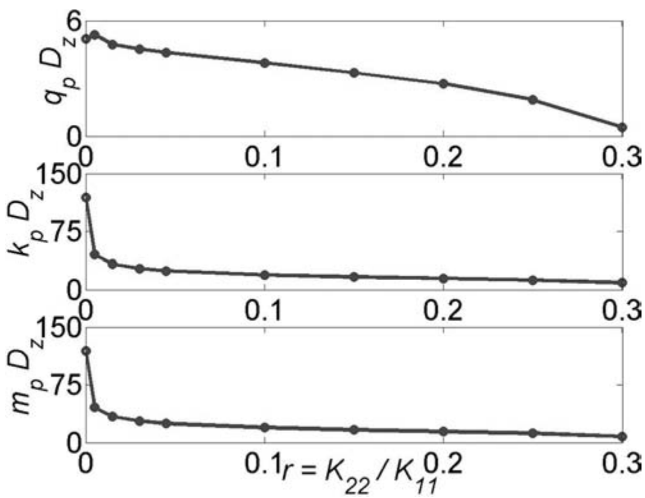

FIGURE 3 The behavior of the reduced wave vectors q_pD_z, k_pD_z, m_pD_z, respectively – starting from the top, is represented as a function of the elastic ratio r in the case of strong anchoring. Note that the critical value of the elastic ratio is $r_c = 0.303$.

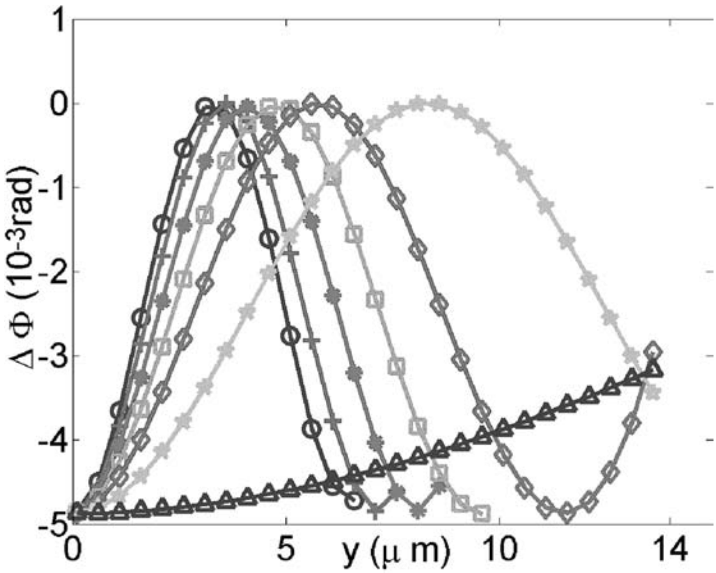

FIGURE 4 $\Delta\Phi$ vs. y for various elastic ratios $r < r_c = 0.303$ in the case of strong anchoring. The in plane distortion period increases with r (Chosen values of $r = 0.0001$; 0.045; 0.10; 0.15; 0.2; 0.25; 0.30).

In Figure 4 the corresponding phase retardation is reported, showing the y-dependence estimated in (14).

The evaluation of the phase retardation has been done also in the case of weak anchoring, for a fixed r value ($r = 0.045$, see Fig. 5). The different anchoring strengths always are given in terms of the relevant extrapolation lengths, affecting through the boundary conditions the coefficients of the dispersion relation (11). The optical phase retardation is modulated and turns out to be strictly dependent on the driving field and on the anchoring strengths. In particular, for the chosen r-values the dependence on the tilt anchoring strength is more effective than on the twist anchoring one; and the period of the phase retardation for weak anchoring is greater than in the case of strong anchoring.

4. CONCLUSIONS

We have analysed the optical features of a initially unidirectional planar cell, where the glass plates were treated in order to provide either strong- or weak anchoring. The cell, filled with a NLC characterized by positive susceptivity anisotropy and small elastic ratio between twist- and splay- elastic

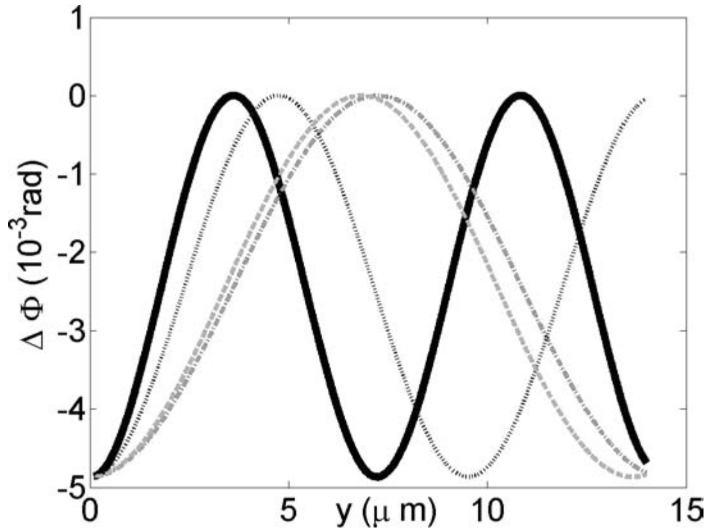

FIGURE 5 $\Delta\Phi$ vs. y for various anchoring strengths with fixed elastic ratio $r = 0.045$. The reduced extrapolation lengths are: ($l_\theta = l_\varphi = 0$, bold line), ($l_\theta = 1$, $l_\varphi = 0$, dashed line), ($l_\theta = 0$, $l_\varphi = 1$, dotted line), ($l_\theta = l_\varphi = 1$, mixed line). Note that for strong anchoring the in-plane distortion is characterized by the minimal periodicity.

constants, was subjected to an external magnetic field normal to the cell walls. The conditions for the arising of a biperiodic distortion allow us to define the cell as a diffraction grating along the in-plane direction of the initial director profile. In such a biperiodic distorted nematic cell optical phase shift measurements can give information related to the different anchoring conditions at the boundary.

In fact, the optical phase retardation $\Delta\Phi$ of a transmitted polarized monochromatic light beam with normal incidence turns out to be a convenient parameter for investigating the properties of the modulated grating, i.e. of the periodic distortion induced by an external magnetic field. The phase difference $\Delta\Phi$ was calculated referring $\Phi(H > H_p)$ to $\Phi_o(H = 0)$ in the approximation of small deformation.

We have found that:

- $\Delta\Phi$ exhibits a periodic pattern vs. the in-plane y-direction;
- the periodic pattern close to the threshold is characterized by the period π/q, corresponding to the 2nd harmonic of the actual in-plane distortion;
- $\Delta\Phi$ dramatically is sensitive to both the external field and the surface anchoring, as it is shown in Figures 4 and 5.

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