Diffraction Gratings in a Nematic Cell Due to Spatial Variation of Surface Order Parameter

D. ANDRIENKO, I. PINKEVICH[*], YU. REZNIKOV
Institute of Physics, 46 Prospect Nauki, Kyiv, Ukraine 252650
[*]Kyiv University, 6 Prospect Glushkova, Kyiv, Ukraine 252000
denis@marion.iop.kiev.ua

The influence of a periodical spatial modulation of a *surface* order parameter on the distribution of the order parameter in a nematic liquid crystal bulk is studied. The problem is treated in the framework of the Landau - de Gennes theory with an anchoring energy in the form $F_S \sim (S-Q)^2$, where S is the NLC order parameter and Q is the surface order parameter. It is shown that the order parameter grating, which damps exponentially with the distance to the cell plates, appears in the cell bulk. The damping coefficient is inversely proportional to the coherence length ξ of the nematic-isotropic phase transition. Diffraction efficiency of this grating is proportional to $(\xi\Delta Q)^2$, where ΔQ is an amplitude of the order parameter modulation, and is sufficient for experimental observations.

Keywords: diffraction gratings, order parameter, aligning surface

INTRODUCTION

The influence of the cell surfaces on the orientational order of nematic liquid crystals (NLC) has been intensely studied over the last decade[1]. It has been reported recently, that the illumination of an aligning surface results in the appearance of an easy orientation axis on this surface[2-4]. Since light can be focused to micrometer-sized pixels, this in principle enables the modulation of the nematic liquid crystal orientation on the cell surfaces with high spatial frequency. Such modulation of an easy axis direction has been studied in papers[6,7]. In[6] was studied the dependence of the effective easy axis on the parameters of modulation. In[7] it was shown that the director gratings appear in the cell bulk due to the modulation of an easy axis direction and the diffraction grating can be recorded.

Optical influencing the director orientation suffers from several drawbacks, however, especially domain orientation of the NLC and appearance of defects due to large distortions of the director on the aligning surfaces.

We propose to change the NLC orientational order by means of controlling its order parameter value on the cell plates. In this case the director orientation is uniform all over the cell and only the NLC order parameter is changed, that makes possible more dense record of the NLC orientation order without defects of orientational structure. In particular, in this paper we consider the influence of the spatially modulated surface order parameter on the bulk distribution of the NLC order parameter. The diffraction efficiency of the appearing grating of the refractive indices is estimated as well.

1. FREE ENERGY OF THE CELL

Let the aligning plates provide the homogeneous homeotropic distribution of the director $\vec{n}$ in the NLC cell. Then the free energy density of the cell can be written as[9,10]

$$f = f_{LG} + f_B + f_S \qquad (1)$$

where f_{LG} is the Landau-de Gennes (LG) free energy density, f_B is the free energy density due to the distortion of the NLC order parameter in the cell bulk, f_S is an anchoring energy.

According to the LG phenomenological model, the free energy density f_{LG} can be expanded in powers of scalar order parameter S

$$f_{LG} = f_i + \tfrac{1}{2}a\left(T - T^*\right)S^2 - \tfrac{1}{3}bS^3 + \tfrac{1}{4}cS^4, \qquad (2)$$

where f_i is the free energy density of the isotropic phase, a, b, c are supposed to be constants, T is the absolute temperature, T^* is the lowest temperature at which the isotropic phase is metastable.

We adopt the hypothesis of small deviations of the order parameter all over the cell from the value S_B in the infinite NLC sample. In this approach the LG free energy density (2) can be replaced by parabolic dependence centered in S_B[11]

$$f_{LG} = f_i + \tfrac{1}{3}\frac{L_1\left(S - S_B\right)^2}{\xi^2}, \qquad (3)$$

where the coherence length ξ of NLC is defined as

$$\xi^2 = \tfrac{2}{3} L_1 \Big/ \left(\partial^2 f_{LG} / \partial S^2\right)_{S=S_B}. \qquad (4)$$

Under the slow variation of the NLC order parameter in a cell bulk and one-elastic-constant approximation the free energy density f_B takes the form[9]

$$f_B = \tfrac{1}{3} L_1 \left(\vec{\nabla} S\right)^2, \qquad (5)$$

where L_1 is an elastic constant which can depend on temperature T and pressure P, but to a good approximation may be considered to be constant.

In the absence of the surface biaxial order, the anchoring energy can be written as[5]

$$f_S = \tfrac{1}{2}\frac{L_1}{L}\mathrm{Tr}\left[\left(S_{\alpha\beta} - Q_{\alpha\beta}\right)^2\right], \qquad (6)$$

where L is an anchoring coherence length, $Q_{\alpha\beta} = Q(\vec{r})\left(e_\alpha e_\beta - \tfrac{1}{3}\delta_{\alpha\beta}\right)$ is the tensorial order parameter of the surface, $\vec{e}$ is the easy axis direction, $S_{\alpha\beta} = S\left(n_\alpha n_\beta - \tfrac{1}{3}\delta_{\alpha\beta}\right)$ is the tensorial order parameter of the NLC.

In our case $\vec{e} = (0,0,\pm 1)$, and the order parameter of the surface is assumed to be spatially modulated along y coordinate with period $\Lambda = 2\pi/q$

$$Q(y) = Q + \Delta Q \sin qy. \qquad (7)$$

Then the Exp. (6) for f_S takes more simple form

$$f_S = \tfrac{1}{2}\tfrac{L_1}{L}\left(S - Q(y)\right)^2. \qquad (8)$$

Equation for the order parameter S with corresponding boundary conditions can be obtained from the minimization of the total free energy of the NLC cell

$$F = \int \left(f_B + f_{LG}\right) dV + \int f_S \, dS, \qquad (9)$$

where f_B, f_{LG}, f_S are defined by the Exps. (3,5,8).

2. DISTRIBUTION OF THE NLC ORDER PARAMETER

After the minimization of the total free energy (9) one can obtain the following equation and boundary conditions for the NLC order parameter S

$$\begin{cases} \xi^2\left(S_{yy}+S_{zz}\right)=S-S_B \\ \left[LS_z \pm \left(S-Q(y)\right)\right]_{z=d,0}=0 \end{cases}, \tag{10}$$

where we denote $S_x=\partial S/\partial x$.

Seeking the solution of the boundary problem (10) in the form

$$S(y,z)=S(z)+\Delta S(z)\sin qy\,, \tag{11}$$

we obtain

$$S(z)=S_B+\frac{\xi}{\alpha}\left(Q-S_B\right)\left\{\sinh\frac{z}{\xi}+\sinh\frac{d-z}{\xi}\right\}, \tag{12}$$

$$\Delta S(z)=\frac{\xi_1\Delta Q}{\beta}\left\{\sinh\frac{z}{\xi_1}+\sinh\frac{d-z}{\xi_1}\right\}, \tag{13}$$

where $\alpha=L\left(\cosh\frac{d}{\xi}-1\right)+\xi\sinh\frac{d}{\xi}$, $\beta=L\left(\cosh\frac{d}{\xi_1}-1\right)+\xi_1\sinh\frac{d}{\xi_1}$, $\xi_1=\xi\big/\sqrt{1+q^2\xi^2}$.

It is seen from expression (11), that the grating of order parameter appears in the NLC bulk with the period $2\pi/q$ of surface order parameter modulation.

According to LG mean field theory, the coherence length ξ have the form $\xi_0\left(T/T^*-1\right)^{-1/2}$, where ξ_0 is a macroscopic length determined by the range of intermolecular forces: $\xi_0\sim 20\,\mathring{A}$. Near the temperature of phase transition to the isotropic state the coherence length is enhanced by a factor 10-20. Since the typical cell thickness $d\geq 1\mu m$, we have, that in the NLC cells $\xi/d<<1$. Taking into account that for the typical NLC cell $q\xi<<1$, the expressions (12,13) can be simplified to

$$S(z)=S_B+\frac{Q-S_B}{1+L/\xi}\exp\left(-d/\xi\right)\left\{\sinh\frac{z}{\xi}+\sinh\frac{d-z}{\xi}\right\}, \tag{14}$$

$$\Delta S(z)=\frac{\Delta Q}{1+L/\xi}\exp\left(-d/\xi\right)\left\{\sinh\frac{z}{\xi}+\sinh\frac{d-z}{\xi}\right\}.$$

Thus, the order parameter grating damps exponentially with the distance to the cell bulk. The dumping constant is inversely proportional to the coherence length ξ.

3. DIFFRACTION ON THE ORDER PARAMETER GRATING

The refractive indices of ordinary and extraordinary light waves in the NLC are, at first order in S

$$n_e^2 = \varepsilon_{iso} + \tfrac{2}{3}\varepsilon_a S\,,\; n_o^2 = \varepsilon_{iso} - \tfrac{2}{3}\varepsilon_a S \tag{15}$$

where $\varepsilon_{iso} = \tfrac{1}{3}\left(\varepsilon_\parallel + 2\varepsilon_\perp\right)$, $\varepsilon_a = \varepsilon_\parallel - \varepsilon_\perp$, $\varepsilon_\parallel, \varepsilon_\perp$ are the main values of the dielectric susceptibility tensor. Thus, the spatial modulation of the order parameter along y coordinate leads to the modulation of the refractive index of NLC and the diffraction grating arises in the cell.

Let a plane light wave be normally incident on the cell plane $z = L$ and be diffracted by this grating. In the cell bulk the light field in the geometrical optics approximation can be written as

$$\vec{E}(y,z) = \vec{E}_0 \exp\left\{i\psi(y,z)\right\}, \tag{16}$$

where $\psi(y,z) = \frac{\omega}{c}\int_L^z n_o(y,z')dz'$, $n_o(y,z)$ is a refractive index of the ordinary light wave. Thus, the phase of the light, passing through the cell is spatially modulated along y coordinate. Diffraction pattern formed by the light field (16) can be found by taking the spatial Fourier transform of this field at the opposite plane z = 0: $\vec{\Phi}(\alpha) = \int_{-\infty}^{\infty} \vec{E}(y,0)\exp(-ik\sin\alpha y)dy$, where α is the angle of deviation of the diffracting light beam from the direction of the incident beam. Since the light field (16) is a periodic function with period $\Lambda = 2\pi/q$, the diffracted field takes the form[12]

$$\vec{\Phi}(\alpha) \sim \frac{\sin\left(\frac{1}{2}\Lambda N k \sin\alpha\right)}{\sin\left(\frac{1}{2}\Lambda k \sin\alpha\right)} \int_{-\Lambda/2}^{\Lambda/2} \vec{E}(y,0)\exp(-ik\sin\alpha y)dy\,, \tag{17}$$

where N is the number of gaps which form the diffraction pattern.

Expanding the light field $\vec{E}(y,0)$ as a power series in ε_a and leaving only the terms linear in ε_a we obtain that in the m-th diffraction maximum

$$\Phi(\alpha) \sim J_m(\delta), \tag{18}$$

where $J_m(x)$ is the Bessel function of integer order m, $\delta = \frac{16\pi}{3} n_{iso} \frac{\varepsilon_a}{\varepsilon_{iso}} \frac{\xi_1^2}{\lambda\beta} \Delta Q \sinh^2 \frac{d}{2\xi_1}$, $n_{iso} = \sqrt{\varepsilon_{iso}}$. Here we take into account, that the condition for the m-th diffraction maximum is $m = (k/q)\sin\alpha$. Thus, the light intensity in the m-th diffraction order is

$$I_m \sim \left|\Phi(\alpha)\right|^2 \sim J_m^2(\delta). \tag{19}$$

The diffraction efficiency of the grating defined as $\eta_m = I_m/I_0$ is $\eta_m = J_m^2(\delta)/J_0^2(\delta)$ and in the $\xi_1/d << 1$ approximation takes the form

$$\eta_1 = \left(\tfrac{16\pi}{3} n_{iso} \frac{\varepsilon_a}{\varepsilon_{iso}} \frac{\xi_1/\lambda}{1 + L/\xi_1} \Delta Q \right)^2 \qquad (20)$$

One can see that the diffraction efficiency of the grating in the cell bulk is proportional to the squared amplitude of the surface order parameter modulation and the ratio of the nematic coherence length to the wave length of incident light.

For typical NLC parameters $n_{iso} \approx 3/2$, $\varepsilon_a \approx 1/10$, $\xi \approx 50\,\mathring{A}$, $\lambda = 500nm$ and for the strong anchoring ($L = 0$) we have $\eta_1 = 10^{-5}(\Delta Q)^2$. In particular, if $\Delta Q = 0.3$, $\eta_1 = 10^{-6}$. But the value η_1 can enhance strongly (100-500 times) near the nematic-isotropic transition point due to the increasing of the coherence length ξ.

We have to compare the obtained diffraction efficiency with the efficiency of light scattering on the fluctuations of the director and the NLC order parameter. The light scattering on the director fluctuations is very intensive. However, we can choose an appropriate geometry of experiment (e.g. with parallel polarization vectors of the incident and scattered light beams) when only the scattering on the fluctuations of order parameter are present. The light scattering intensity on the fluctuations of order parameter in the nematic phase has the same order of magnitude as the light scattering intensity in the isotropic phase[13]. The last can be estimated from the differential cross section (per unit solid angle, per unit square) of the light scattered on the order parameter fluctuations[14]

$$\frac{d\sigma}{Sd\Omega} = \frac{2\pi^2 d\varepsilon_a}{9\lambda^4 L_1} k_B T \xi^2$$

For typical NLC parameters $L_1 \approx 5 \times 10^{-7} dyn$, $\xi \approx 50\,\mathring{A}$ we obtain $\frac{d\sigma}{Sd\Omega} \sim 10^{-7} - 10^{-8}$, thus the intensity of the light, scattered on the fluctuations of order parameter can be far less then the intensity of the diffracted beam.

4. CONCLUSIONS

We have studied the influence of the surface order parameter modulation on the nematic liquid crystal ordering in the cell bulk. It was shown, that the spatial modulation of the surface order parameter with period $2\pi/q$ induces the grating of the bulk NLC order parameter with the same period, exponentially damping toward the NLC bulk with the damping coefficient inversely proportional to the nematic - isotropic coherence length ξ. The NLC order parameter grating causes the grating of the refractive indices, and thus, the diffraction grating appears in the NLC bulk. The diffraction efficiency of this grating is proportional to the squared amplitude of the surface order parameter modulation ΔQ and squared ratio of the re-normalized coherence length $\xi_1 = \xi / \sqrt{1+(q\xi)^2}$ to the wavelength of the diffracting light and depends on the anchoring coherence length *L*. Estimations carried out for typical NLC parameters show that the value of the diffraction efficiency is sufficient for experimental observations.

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