Doctopic: Optical physics ARTICLE IN PRESS PLA:17877

Physics Letters A ●●● (●●●●) ●●●–●●●

Contents lists available at ScienceDirect

Physics Letters A

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Director reorientation in twisted nematic liquid crystals due to thermomechanical effect

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A R T I C L E I N F O

Article history:
Received 17 March 2008
Received in revised form 17 April 2008
Accepted 22 April 2008

Communicated by V.M. Agranovich

PACS:
61.30.-v
65.40.Df

Keywords:
Twisted nematic liquid crystals
Director reorientation
Temperature gradient

A B S T R A C T

We have studied molecular director reorientation in a twisted nematic liquid crystal induced by a two-dimensional temperature gradient. We studied the effect of rate change between the temperature gradients in two directions. Our obtained director reorientations are in the range that can be observed experimentally very easily.

1. Introduction

Thermal effects in nematic liquid crystals (NLC) have been the goal of many researches, particularly owing to temperature dependence of the physical parameters of nematic liquid crystal as mass density, order parameter, index of refraction [1,2], Frank's free elastic energy constants and so on [3], but almost of them are significant in some special cases and in many cases are ignorable. Among them the most important thermal changes occur due to thermomechanical effect in nematic liquid crystals that can deduce larger effects in NLC than other effects [4].

Thermomechanical effects for cholesteric liquid crystals have been investigated largely experimentally and theoretically, where these effects are related to the absence of left–right symmetry of the director in the cholesterics [5]. It was shown that these effects have some analogues in nematic LCs [4]. Three principle thermomechanical effects have been introduced in [4]; first one is hydrodynamical flow due to temperature gradient, second one is the onset of temperature drop due to nonuniform flow and third type is additional director deflection due to temperature gradient. By variation of dissipation function introduced in [4] we can find equations that describe all the mentioned effects. However, we have to note that the work done by thermomechanical forces does not change to heat, but it changes to kinetic energy of a rotation flow (e.g. via direct thermomechanical effect) [6]. Thermomechanical effects have been investigated theoretically and experimentally, widely [4,6–12]. These effects require nonuniform director distribution, intrinsically. Thermomechanical effect in hybrid and cylindrical–hybrid orientation has been investigated in [6–9] theoretically and experimentally. It is shown that with usual vertical thermal differences (5–10 K) in a usual cell of thickness 100 μm we will have hydrodynamical flow in the range of 1 μm/s. Oscillatory motions of "flexible ribbon" due to hydrodynamical flow were shown in [10]. Hydrodynamical flow for the homeotropic NLC induced by light field [11] and planar NLC induced by quasistatic electrical field was shown theoretically and experimentally in [12]. Thermomechanical effect on the significant lowering of the optical Freedericksz transition (OFT) in dye-doped nematic liquid crystals was shown in [13].

In this work we will consider the director reorientation due to the third thermomechanical effect in a two-dimensional temperature gradient in a plane parallel to the boundary surfaces which can be caused by any external heat sources as Peltie element or light absorption in nematic liquid crystal as well. In the case of temperature gradient due to light absorption, dye-doped nematic liquid crystals will show larger temperature gradients and consequently larger director reorientations. These director reorientations will create additional torque which acts on the director simultaneously with other torques and stabilizes or destabilizes them.

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doi:10.1016/j.physleta.2008.04.052

Please cite this article in press as: J.B. Poursamad, R.S. Hakobyan, Director reorientation in twisted nematic liquid crystals due to thermomechanical effect, Physics Letters A (2008), doi:10.1016/j.physleta.2008.04.052

The present work is organized as follows. In Section 2 we will find dominant equation of the director reorientation for twisted nematic liquid crystals with strong anchoring conditions at the boundaries, by perturbations linearization and we will find an analytical answer in the steady-state case. In Section 3 we will solve the found perturbational differential equation numerically and will give some approximations of director reorientations in a two-dimensional temperature gradient. Finally in Section 4 we will have some discussion about the found results.

2. Thermomechanical equation of director reorientation

We have considered a NLC layer as Fig. 1. Initially director lies on the xy plane with no component in the z direction, where a Cartesian coordinate system is considered. We described $\theta(z) = \pi z/2L$ the angle between the director and x axis, and then initial director will be $\hat{n}(\vec{r}) = \cos(\theta(z))\hat{e}_x + \sin(\theta(z))\hat{e}_y$, where $\hat{e}_x$ and $\hat{e}_y$ are unit vectors in x and y directions consequently. We have $\hat{n}(z=0) = \hat{e}_x$ and $\hat{n}(z=L) = \hat{e}_y$, where L is the cell thickness. Equation for director equilibrium orientation can be found from Euler–Lagrange–Rayleigh variational method [14]:

$$\Pi_{ij}\left[\frac{\delta R}{\delta(\partial n_i/\partial t)} - \frac{\partial}{\partial x_k}\frac{\delta R}{\delta(\partial^2 n_i/\partial x_k \partial t)} + \frac{\partial F}{\partial n_i} - \frac{\partial}{\partial x_k}\frac{\delta F}{\delta(\partial n_i/\partial x_k)}\right] = 0, \tag{1}$$

where

$$F = \frac{1}{2}K_1(\operatorname{div}\hat{n})^2 + \frac{1}{2}K_2(\hat{n}\,.\,curl\,\hat{n})^2 + \frac{1}{2}K_3(\hat{n}\times curl\,\hat{n})^2 \tag{2}$$

is Frank's free energy density and K_1, K_2 and K_3 are Frank's constants for splay, twist and bend consequently. The projection operator $\Pi_{ij} = \delta_{ij} - n_i n_j$ ensures conservation of normalization $\hat{n}^2 = 1$ and

$$R = R^{\mathrm{VISC}} + R^{\mathrm{TM}} \tag{3}$$

and

$$R^{\mathrm{VISC}} = \frac{1}{2}\gamma\left(\frac{\partial \hat{n}}{\partial t}\right)^2. \tag{4}$$

Here γ (Poise) is the viscosity constant. We note that in viscous dissipation function R^{VISC} we have neglected the relationship of the director to the hydrodynamic degrees of freedom [14], and R^{TM} is the thermomechanical dissipation function introduced in [4]. Because of the complexity of the relations for twisted nematic liquid crystals, we have used the single constant approximation for Frank constants: $K_1 = K_2 = K_3 = K$, then [15]

$$\frac{\partial F}{\partial n_i} - \frac{\partial}{\partial x_k}\frac{\delta F}{\delta(\partial n_i/\partial x_k)} = -K\nabla^2 n_i \tag{5}$$

and the thermomechanical "force" generated by the dissipation function is

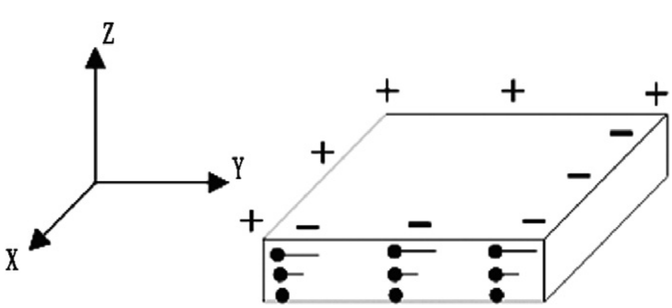

Fig. 1. Geometry of twisted nematic liquid crystal with a two-dimensional temperature gradient.

$$\begin{aligned} f_j^{\mathrm{TM}} &= \frac{\delta R^{\mathrm{TM}}}{\delta(\partial n_i/\partial t)} \\ &= \frac{1}{2}(2\xi_1 - \xi_3)\vec{\nabla}_i T \operatorname{div}\hat{n} - \xi_2(\hat{n}\,.\,curl\,\hat{n})[\hat{n}\times\vec{\nabla}]_i T \\ &\quad + \xi_3 m_{ik}\vec{\nabla}_k T - (\xi_3 - \xi_4)m_{ik}n_k(\hat{n}\,.\,\vec{\nabla})T \end{aligned} \tag{6}$$

where

$$m_{ik} = \frac{1}{2}\left(\frac{\partial n_i}{\partial x_k} + \frac{\partial n_k}{\partial x_i}\right) \tag{7}$$

is the symmetric tensor of director gradient, ξ_i (in erg/K cm) are the thermomechanical coefficients, $T(x,y)$ is two-dimensional local temperature. In our calculation we consider the director distribution homogeneous in the xy plane, so $\partial/\partial x = \partial/\partial y = 0$ and we linearize our relations by the perturbation $\delta\hat{n}$: $\hat{n} = \hat{n}^\circ + \delta\hat{n}(\hat{n}^\circ\,.\,\delta\hat{n} = 0)$.

After a cumbersome calculation we will get the generation of a new component for director in the z direction due to the thermomechanical effect. Normalized equation for the director z component has the form

$$\frac{\partial^2 \delta n_z(Z,\tau)}{\partial Z^2} + \delta n_z(Z,\tau) + \sin(Z)\frac{\partial\Theta}{\partial X} - \cos(Z)\frac{\partial\Theta}{\partial Y} = \frac{\partial \delta n_z(Z,\tau)}{\partial\tau}, \tag{8}$$

where Z is normalized coordinate $Z = \pi z/2L$, $X = x/L$, $Y = y/L$ and $\tau = t/4\tau_r$, with electrical relaxation time (due to the giant optical nonlinearity) $\tau_r = \frac{\gamma L^2}{\pi^2 K}$ [14] and

$$\Theta = \frac{2L}{\pi K}\left(\xi_2 + \frac{1}{2}\xi_3\right)T(x,y). \tag{9}$$

For the steady-state case $(\partial/\partial\tau = 0)$ with the strong anchoring conditions at the interfaces: $\delta n_z(0,\tau) = \delta n_z(L,\tau) = 0$, we will have

$$\begin{aligned} \delta n_z(z) = \frac{L(\xi_2 + \frac{1}{2}\xi_3)}{2K}\Bigg(&\frac{z}{L}\cos\left(\frac{\pi z}{2L}\right)\frac{\partial T(x,y)}{\partial x} \\ &+ \left(\frac{z}{L} - 1\right)\sin\left(\frac{\pi z}{2L}\right)\frac{\partial T(x,y)}{\partial y}\Bigg). \end{aligned} \tag{10}$$

It shows that the reorientation of director due to thermomechanical effect linearly depends on the cell thickness L and the interplay between the temperature gradients in x and y directions. Here we have shown the steady-state case for different situations which can occur (see Fig. 2). We have used the parameters of NLC **5CB** $K \approx 6.3\times 10^{-7}$ (erg/cm), $L = 10^{-2}$ cm, $\xi_2 \approx \xi_3 \approx 10^{-6}$ erg/K cm [4].

We observe from this figure that as α $(\partial T/\partial y = \alpha\,\partial T/\partial x)$ is smaller the effects of the temperature gradient in y direction are smaller and the effects due to the temperature gradient in x direction are dominant. For the case with no temperature gradient in

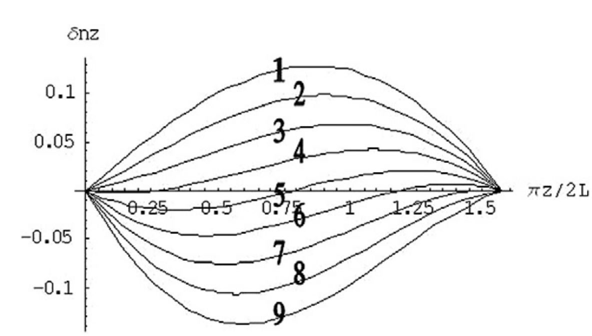

Fig. 2. New generated component of the director across the nematic liquid cell for different case of the temperature gradient distribution $\partial T/\partial y = \alpha\,\partial T/\partial x$, $(\partial T/\partial x = 30$ K/cm): 1$(\alpha = 0)$, 2$(\alpha = 0.25)$, 3$(\alpha = 0.5)$, 4$(\alpha = 0.75)$, 5$(\alpha = 1)$, 6$(\alpha = 1.25)$, 7$(\alpha = 1.5)$, 8$(\alpha = 1.75)$, 9$(\alpha = 2)$.

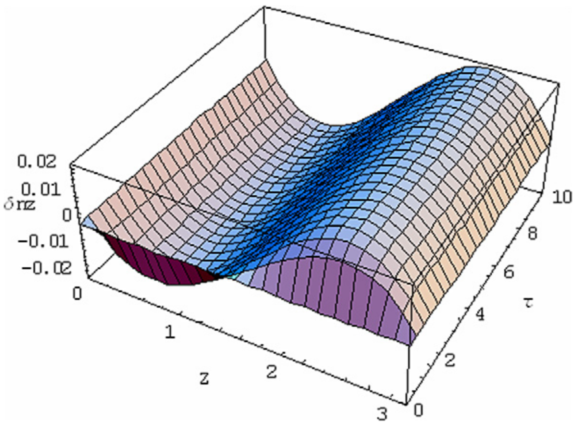

Fig. 3. Numerical solution of δn_z vs normalized Z and τ for the case that $dT/dx = 30$ and $\alpha = 1$ with symmetric halves before and after $z = L/2$ in opposite directions.

y direction we have a maximum $\delta n_z \approx 0.13$ for $dT/dx = 30$ K/cm approximately at the middle of the cell ($z \approx 0.55L$). But as the temperature gradient in the y direction increases the height of the maximum reorientation decreases with pulling the maximum to the upper interface ($z = L$) of the cell, approximately when $\alpha \approx 0.75$ the curve contacts the horizontal axis near the lower interface ($z = 0$), when $\alpha = 1$ the curve contacts horizontal axis at the middle ($z = L/2$) and we have symmetric case in upper and lower halves of the cell with equal reorientation but in opposite directions, for larger α's the effect of the temperature gradient in y direction dominates; for the cases $\alpha \geqslant 1.5$ the curve does not coincide with the horizontal axis and we will have the new generated component of the director only in the lower half of the space.

3. Numerical solution

We are able to solve Eq. (8) for director reorientation caused by temperature gradient with the boundary (strong anchoring) and initial conditions $\delta n_z(0, \tau) = \delta n_z(L, \tau) = \delta n_z(Z, 0) = 0$ using "Mathematica5.1". In this calculation we used parameters of NLC **5CB**.

Fig. 3 shows three-dimensional picture of new generated component of the director which in this special case will be averagely zero across the whole cell.

Fig. 4 shows the saturation of the new component of the director. If we fit this figure with relation $\delta n_z = \delta n_z^{\text{steady-state}}(1 - e^{(-t/\tau_{\text{th}})})$ we will see the rise time of the director for thermomechanical reorientation $\tau_{\text{th}} = \chi \tau_r$, where $\chi \approx 1.5$. If we assume that ϑ is the average deviation angle from xy plane ($\delta n_z = \sin \vartheta$), we will have $\vartheta_1 \approx 5°$, $\vartheta_2 \approx 3.5°$, $\vartheta_3 \approx 1.7°$, $\vartheta_4 \approx -1.7°$, $\vartheta_5 \approx -3.5°$ and $\vartheta_6 \approx -5°$. These average deviations show that as the rate of temperature gradient between x and y directions change molecules of liquid crystal change their directions up to down or vise versa. It should be noted that we neglected here from temperature dependence of the material parameters for simplicity, so used $\Delta T_{\max}$ must be not too large, otherwise their temperature dependence must be coupled with thermomechanical ones properly. However, the used temperature gradients are obtainable with a few changes in the temperature of the nematic liquid crystal in the case of light absorption.

4. Conclusion

We calculated director reorientation relation under a two-dimensional temperature gradient with the help of thermomechanical effect when the temperature gradients are parallel to the boundary surfaces. We found that the temperature gradient in one direction will oppose to the director reorientation induced by the next temperature gradient, so as their difference is larger, the director reorientation the larger, but it must not too large to produce turbulence in the medium. Thermomechanical reorientations are proportional to cell thickness and thermomechanical coefficients magnitude, linearly. Our calculated director reorientations are comparable with the reorientations due to giant optical nonlinearity [14] and so can deduce comparable nonlinear effects in nematic liquid crystals as self-focusing or self-defocusing, self-diffraction and so on.

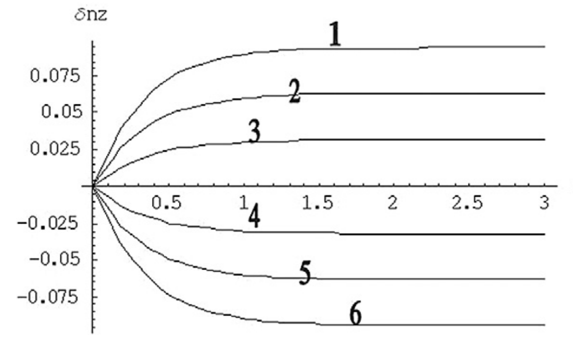

Fig. 4. Two-dimensional profile of δn_z vs normalized $\tau(\partial T/\partial x = 30)$: $1(\alpha = 0.25)$, $2(\alpha = 0.5)$, $3(\alpha = 0.75)$, $4(\alpha = 1.25)$, $5(\alpha = 1.5)$ and $6(\alpha = 1.75)(\partial T/\partial y = \alpha \partial T/\partial x)$.

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Please cite this article in press as: J.B. Poursamad, R.S. Hakobyan, Director reorientation in twisted nematic liquid crystals due to thermomechanical effect, Physics Letters A (2008), doi:10.1016/j.physleta.2008.04.052