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GENERAL THRESHOLD PROPERTIES OF LIQUID CRYSTAL SLAB WITH WEAK ANCHORING BOUNDARIES

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Abstract On the basis of the Rapini-Papoular anchoring energy unifying the azimuthal and polar angle anchorings, the general surface torque balance equations for field-controlled twisted chiral nematic liquid crystal cells with weak anchoring boundary coupling have been derived analytically. The relationship between the anchoring energy and the threshold field of Fréedericksz transition has been discussed rigorously.

INTRODUCTION

Surface effects on the director configuration in nematic liquid crystal (NLC) cells have been widely studied for a long time. In most practical conditions the surface forces are not strong enough to impose a well-defined director orientation. To describe a weak anchoring surface from an untwisted NLC sample, Rapini and Papoular¹ (R-P) have introduced a simple phenomenological expression for the interfacial energy per unit area for a one-dimensional deformation

$$g_s = \frac{A}{2} \sin^2(\theta^\circ - \theta_0), \quad (1)$$

where θ_0 is the tilt angle for the easy direction \underline{e} , and θ° is the preferred tilt of the director at the nematic-wall interface. The anchoring strength or anchoring energy proportionality constant, A , determines the ability of the director to deviate from the easy direction. For a twisted NLC sample the R-P energy density must be extended to the more general form as²

$$g_s = -\frac{A}{2} (\underline{n} \cdot \underline{e})^2, \quad (2)$$

which is a non-linear combination of the azimuthal and polar angles. On the basis of the R-P function, some investigators have studied the influence of the bulk orientation of NLC by an interfacial effect^{3–10} and have attempted^{11–12} to measure A .

However, in the previous studies³⁻¹⁰, the unified R-P energy form Eq.(2) has been written as a linear combination of an azimuthal angle anchoring term $g_s(\theta)$ and a polar one $g_p(\phi)$. Although such a separation simplifies the mathematical analysis, there is no physical reason to make such a separation. Since the proposal of Eq.(2), the calculation of the field-controlled director orientation in a twisted chiral nematic (TCN) slab with weak anchoring has been an open question for more than 20 years.

In this paper we give a report on the general Fréedericksz transition of the problem.

TORQUE BALANCE EQUATIONS

We consider a nematic cell located between the two planes $z = 0$ and $z = d$ with mirror symmetry with respect to the middle plane $z = d/2$, where d is film thickness. The surface tilt angle, θ° , is taken to be the same on both surfaces. The easy direction \underline{e} on the surface of $z = 0$ and the director in the slab may be expressed as

$$\underline{e} = (\cos \theta_o, 0, \sin \theta_o), \quad (3)$$

$$\underline{n} = (\cos \theta \cos \phi, \cos \theta \sin \phi, \sin \theta), \quad (4)$$

respectively, where the polar angle ϕ and tilt angle θ are functions of z and the latter is measured from the slab plane. If a magnetic field $\underline{H} (= (0, 0, H))$ is applied to the TCN cell, the free energy density in the bulk may be expressed as¹³

$$\begin{aligned} g_b &= \frac{k_{11}}{2}(\nabla \cdot \underline{n})^2 + \frac{k_{22}}{2} \left(\underline{n} \cdot \nabla \times \underline{n} + \frac{2\pi}{p_o} \right)^2 + \frac{k_{33}}{2} [\underline{n} \times (\nabla \times \underline{n})]^2 - \frac{\Delta\chi}{2} (\underline{n} \cdot \underline{H})^2 \\ &= \frac{1}{2} [f(\theta)\theta^{(1)2} + h(\theta)\phi^{(1)2}] - \frac{2\pi}{p_o} k_{22}\phi^{(1)} \cos^2 \theta + \frac{2\pi^2 k_{22}}{p_o^2} - \frac{\Delta\chi}{2} H^2 \sin^2 \theta, \end{aligned} \quad (5)$$

where $\theta^{(1)} = d\theta/dz$, $\phi^{(1)} = d\phi/dz$, and

$$f(\theta) = k_{11} \cos^2 \theta + k_{33} \sin^2 \theta \quad (6)$$

$$h(\theta) = (k_{22} \cos^2 \theta + k_{33} \sin^2 \theta) \cos^2 \theta. \quad (7)$$

The constants k_{11} , k_{22} , and k_{33} are the splay, twist, and bend elastic constants of the NLC, respectively, p_o denotes the pitch of the material induced by a chiral dopant, and $\Delta\chi$ is the anisotropy of the diamagnetic susceptibility of the NLC.

The total free energy is the sum of the surface energy (Eq.(2)) and the bulk free energy (the integration of Eq.(5) over the cell volume). Applying a new variational calculation for the two dimensional problem¹⁴ to the total free energy, we find four equations describing the equilibrium deformation of the director:

$$\begin{aligned} h(\theta)\phi^{(1)} \Big|_{z=0} &= \frac{2\pi k_{22}}{p_o} \cos^2 \theta \\ &\quad + A(\cos \theta_o \cos \theta \cos \phi + \sin \theta_o \sin \theta) \cos \theta_o \sin \phi \cos \theta, \end{aligned} \quad (8)$$

$$\begin{aligned} f(\theta)\theta^{(1)} \Big|_{z=0} &= A(\sin \theta_o \sin \theta + \cos \theta_o \cos \theta \cos \phi)(\cos \theta_o \sin \theta \cos \phi \\ &\quad - \sin \theta_o \cos \theta), \end{aligned} \quad (9)$$

$$\phi^{(1)} = \frac{1}{h(\theta)} \left(C_1 + \frac{2\pi k_{22}}{p_o} \cos^2 \theta \right), \quad (10)$$

$$f(\theta)\theta^{(1)2} + \frac{1}{h(\theta)} \left(C_1 + \frac{2\pi k_{22}}{p_o} \cos^2 \theta \right)^2 + \Delta\chi H^2 \sin^2 \theta = C_2, \quad (11)$$

where $\theta^{(2)} = d\theta^{(1)}/dz$, and C_1 and C_2 are two constants of integration. Eqs. (8) and (9) are the boundary conditions due to the balance of the torque for twist and tilt, respectively at $z = 0$. Eqs. (10) and (11) give the director orientation in the bulk. The surface torque balance equations at $z = d$ are simply equal to the negative of the right-hand side of Eqs. (8) and (9). Essentially, Eqs.(8)-(11) are the basic equations for solving the threshold problem analytically.

The right-hand side of torque equations (8) and (9) are both functions of ϕ and θ simultaneously. This is entirely different from the corresponding equations obtained in Refs.[5-10], in which one depends only on θ and the other depends only on ϕ . This shows that the challenging problem for the present analysis is to solve the complicated equations (8) and (9).

Under the extreme condition for θ at the midplane of the cell,

$$\theta^{(1)} \left(z = \frac{d}{2} \right) = 0, \quad \theta \left(z = \frac{d}{2} \right) = \theta_M, \quad (12)$$

the constant of integration C_2 in Eq.(11) is determined as

$$C_2 = \frac{1}{h(\theta_M)} \left(C_1 + \frac{2\pi k_{22}}{p_o} \cos^2 \theta_M \right)^2 + \Delta\chi H^2 \sin^2 \theta_M. \quad (13)$$

Using Eq.(13), the integration of Eq.(11) gives

$$\frac{d}{2} = \int_{\theta^o}^{\theta_M} N^{\frac{1}{2}}(\theta) d\theta, \quad (14)$$

where $N^{\frac{1}{2}}(\theta)$ is

$$N^{\frac{1}{2}}(\theta) = f^{\frac{1}{2}}(\theta) \left[\Delta\chi H^2 (\sin^2 \theta_M - \sin^2 \theta) + \frac{1}{h(\theta_M)} \left(C_1 + \frac{2\pi k_{22}}{p_o} \cos^2 \theta_M \right)^2 - \frac{1}{h(\theta)} \left(C_1 + \frac{2\pi k_{22}}{p_o} \cos^2 \theta \right)^2 \right]^{-\frac{1}{2}}. \quad (15)$$

Using Eq.(15) with the mirror symmetry with respect to $z = d/2$,

$$\phi \left(z = \frac{d}{2} \right) = \frac{1}{2} \phi_t, \quad (16)$$

integration of Eq.(10) gives

$$\frac{\phi_t}{2} - \phi^o = \int_{\theta^o}^{\theta_M} \frac{N^{\frac{1}{2}}(\theta)}{h(\theta)} \left(C_1 + \frac{2\pi k_{22}}{p_o} \cos^2 \theta \right) d\theta, \quad (17)$$

where ϕ_t is the difference between the easy directions at the top and bottom surfaces, called the pretwist angle of the cell, and ϕ° is the actual director orientation at the surface deviating from the pretwist direction. Substituting Eq.(10) in the boundary conditions of Eq.(8), we can obtain following the constant of integration C_1

$$C_1 = A(\cos \theta_o \cos \theta^\circ \cos \phi^\circ + \sin \theta_o \sin \theta^\circ) \cos \theta_o \sin \phi^\circ \cos \theta^\circ. \quad (18)$$

Substituting Eqs.(11)(13) in Eq.(9) and using Eq.(15), the final important expression is obtained as

$$f(\theta^\circ)N^{-\frac{1}{2}}(\theta^\circ) = A(\sin \theta_o \sin \theta^\circ + \cos \theta_o \cos \theta^\circ \cos \phi^\circ)(\cos \theta_o \sin \theta^\circ \cos \phi^\circ - \sin \theta_o \cos \theta^\circ). \quad (19)$$

It is clear now that for given values of ϕ_t , θ_o , and H , the values of ϕ° , θ° , and θ_M can be determined completely from Eqs.(14) and (17)-(19).

FRÉEDERICKSZ TRANSITION

To derive the threshold magnetic field H_F of the Fréedericksz transition, we need to suppose $\theta_o = 0$ and $\theta^\circ = \theta_M = 0$ for $H < H_F$ and $\theta_M \rightarrow 0$ when $H \rightarrow H_F$. Because $\theta \leq \theta_M$, to simplify calculations we introduce two new parameters α and α° defined by

$$\sin \alpha = \frac{\sin \theta}{\sin \theta_M}, \quad \sin \alpha^\circ = \frac{\sin \theta^\circ}{\sin \theta_M}. \quad (20)$$

Using the conditions at the Fréedericksz transition and the above parameters, Eqs.(6)(7)(15)(18) can be changed to

$$f(\theta) = k_{11}(1 + \eta \sin^2 \theta_M \sin^2 \alpha), \quad (21)$$

$$h(\theta) - h(\theta_M) = \psi(\sin^2 \theta_M - \sin^2 \theta), \quad (22)$$

$$N^{\frac{1}{2}}(\theta) = \frac{1}{\sin \theta_M \cos \alpha} \sqrt{\frac{k_{11}(1 + \eta \sin^2 \theta_M \sin^2 \alpha)}{\Delta \chi H^2 + S}}, \quad (23)$$

$$C_1 = A \sin \phi^\circ \cos \phi^\circ, \quad (24)$$

respectively, where

$$\eta \equiv \frac{k_{33} - k_{11}}{k_{11}},$$

$$\psi \equiv 2k_{22} - k_{33} + (k_{33} - k_{22})(\sin^2 \theta_M + \sin^2 \theta),$$

$$S \equiv \frac{1}{h(\theta_M)h(\theta)} \left\{ \psi \left(C_1 + \frac{2\pi k_{22}}{p_o} \right)^2 - \frac{4\pi k_{22}}{p_o} \left(C_1 + \frac{2\pi k_{22}}{p_o} \right) [h(\theta_M) + \psi \sin^2 \theta_M] + \left(\frac{2\pi k_{22}}{p_o} \right)^2 [h(\theta_M)(\sin^2 \theta_M + \sin^2 \theta) + \psi \sin^4 \theta_M] \right\}.$$

With these boundary conditions, viz. Eqs.(21)-(24), the limiting integrals in Eqs.(14)(17) can be solved analytically to give the relationship between the threshold

field and the anchoring energy. Using Eqs.(20)-(24), Eqs.(14)(17) at the Fréedericksz transition can be analytically integrated as

$$\begin{aligned} \frac{d}{2} &= \int_{\alpha^\circ}^{\frac{\pi}{2}} \sqrt{\frac{k_{11}(1 + \eta \sin^2 \theta_M \sin^2 \alpha)}{\Delta \chi H^2 + S}} \frac{d\alpha}{\sqrt{1 - \sin^2 \theta_M \sin^2 \alpha}} \\ &= \left(\frac{\pi}{2} - \alpha^\circ\right) k_{11}^{\frac{1}{2}} \left\{ \Delta \chi H_F^2 + \frac{1}{k_{22}^2} \left[\psi_0 \left(C_1 + \frac{2\pi k_{22}}{p_0} \right)^2 \right. \right. \\ &\quad \left. \left. - \frac{4\pi k_{22}^2}{p_0} \left(C_1 + \frac{2\pi k_{22}}{p_0} \right) \right] \right\}^{-\frac{1}{2}}, \end{aligned} \quad (25)$$

and

$$\begin{aligned} \frac{\phi_t}{2} - \phi^\circ &= \int_{\alpha^\circ}^{\frac{\pi}{2}} \frac{(C_1 + 2\pi k_{22} \cos^2 \theta / p_0) N^{\frac{1}{2}}(\theta)}{h(\theta)} \frac{\sin \theta_M \cos \alpha d\alpha}{\sqrt{1 - \sin^2 \theta_M \sin^2 \alpha}} \\ &= \left(\frac{\pi}{2} - \alpha^\circ\right) \left(\frac{C_1}{k_{22}} + \frac{2\pi}{p_0}\right) k_{11}^{\frac{1}{2}} \left\{ \Delta \chi H_F^2 + \frac{1}{k_{22}^2} \left[\psi_0 \left(C_1 + \frac{2\pi k_{22}}{p_0} \right)^2 \right. \right. \\ &\quad \left. \left. - \frac{4\pi k_{22}^2}{p_0} \left(C_1 + \frac{2\pi k_{22}}{p_0} \right) \right] \right\}^{-\frac{1}{2}}, \end{aligned} \quad (26)$$

respectively, where $\psi_0 \equiv 2k_{22} - k_{33}$. Substituting for C_1 and $\pi/2 - \alpha^\circ$ from Eqs.(24) and (25), respectively, Eq.(26) can be calculated to give the following simple expression

$$\phi_t - 2\phi^\circ - \frac{2\pi d}{p_0} = \frac{Ad}{k_{22}} \sin \phi^\circ \cos \phi^\circ. \quad (27)$$

Equation (27) shows the rigorous and important relationship between the anchoring energy and the pretwist angle.

Next we try to derive analytically the threshold field of the Fréedericksz transition. We can obtain from Eqs.(24)(25)(27) the following formula

$$\cot \alpha^\circ = \tan \left[\frac{d}{2} \sqrt{\frac{\Delta \chi H_F^2 + \psi_0(\phi_t - 2\phi^\circ)^2/d^2 - 4\pi k_{22}(\phi_t - 2\phi^\circ)/(dp_0)}{k_{11}}} \right]. \quad (28)$$

Using Eqs.(21)-(24), Eq.(19) changes at the Fréedericksz transition to

$$A \cos^2 \phi^\circ = \sqrt{k_{11} \left[\Delta \chi H_F^2 + \frac{\psi_0(\phi_t - 2\phi^\circ)^2}{d^2} - \frac{4\pi k_{22}(\phi_t - 2\phi^\circ)}{dp_0} \right]} \cot \alpha^\circ. \quad (29)$$

Substituting Eq.(28) in Eq.(29), the threshold magnetic field H_F is given as

$$H_F = \sqrt{\frac{d^2 R + (\phi_t - 2\phi^\circ)[(k_{33} - 2k_{22})(\phi_t - 2\phi^\circ) + 4\pi d k_{22}/p_0]}{\Delta \chi d^2}}, \quad (30)$$

where R and ϕ° are the solutions of the transcendental equations

$$A \cos^2 \phi^\circ = \sqrt{k_{11} R} \tan \left[\frac{d}{2} \sqrt{\frac{R}{k_{11}}} \right], \quad (31)$$

$$\phi_t - 2\phi^\circ - \frac{2\pi d}{p_0} = \frac{Ad}{k_{22}} \sin \phi^\circ \cos \phi^\circ. \quad (32)$$

Equations (30)-(32) are essential and rigorous expressions to derive the threshold magnetic field H_F of the Fréedericksz transition for the TCN cell.

DISCUSSION

In order to compare our results with previous studies, we consider Eqs.(30)-(32) for the threshold property. It is convenient to introduce the dimensionless coupling parameter

$$\lambda = \frac{\pi k_{22}}{Ad}, \quad (33)$$

and also to use the reduced magnetic field $u' = H/H_c$, where

$$H_c = \frac{\pi}{d} \sqrt{\frac{k_{11}}{\Delta\chi}} \quad (34)$$

is the threshold magnetic field for an untwisted nematic slab ($\phi_t = 0$) with rigid boundary coupling ($\lambda = 0$, i.e., $A \rightarrow \infty$).

For this limit, Eq.(30) reduces to

$$H_F d = \sqrt{\frac{k_{11}\pi^2 + (k_{33} - 2k_{22})\phi_t^2 + 4\pi d k_{22}\phi_t/p_o}{\Delta\chi}}. \quad (35)$$

This recovers the result obtained by Becker et al.⁹ under the assumption of strong azimuthal anchoring and the consideration of polar anchoring only. This is also the result reported by Hirning et al.¹⁰ in treating the tilt anchoring and twist anchoring independently and taking both anchoring strengths as infinite. In the case of TN with strong anchoring and $d/p_o = 0$, Eq.(35) reduces to

$$H_F d = \sqrt{\frac{k_{11}\pi^2 + (k_{33} - 2k_{22})\phi_t^2}{\Delta\chi}}. \quad (36)$$

This is the same result as that derived by Leslie³ and Schadt and Helfrich⁴. Furthermore, for the homogeneous nematic slab with weak anchoring, $d/p_o = 0$ and $\phi_t = 0$, Eqs. (30)-(32) lead to

$$A = \sqrt{k_{11}\Delta\chi} H_F \tan \left[\frac{d}{2} \sqrt{\frac{\Delta\chi}{k_{11}}} H_c \right], \quad (37)$$

which is the same as that obtained by Rapini and Papoular¹. These agreements for various limiting conditions offer a good check on the present general theory. However, in order to demonstrate the difference between the present theory and previous studies, it is necessary to consider other special cases.

For an isotropic surface ($\lambda \rightarrow \infty$, $A = 0$), in other words when there is no anchoring energy, we have

$$\Delta\chi H_F^2 = k_{33} \left(\frac{2\pi}{p_o} \right)^2. \quad (38)$$

This provides a reasonable result that the Freedericksz transition does not exist for a nematic slab ($p_o \rightarrow \infty$) coupling with an isotropic surface. We have also calculated numerically the λ dependencies of the threshold field for a 90° twisted slab with the same material parameters as those used in Ref.[9], i.e., $k_{33}/k_{11} = 1.5$, $k_{22}/k_{11} = 0.6$, and $d/p_o = 0$. The results are shown in Fig. 1, where the solid lines give the results for the present calculations and the dashed line is that reported in Ref.[9]. It is clear from Fig.1 that the results of the previous studies may give the correct threshold fields only in the limiting case of $A \rightarrow \infty$.

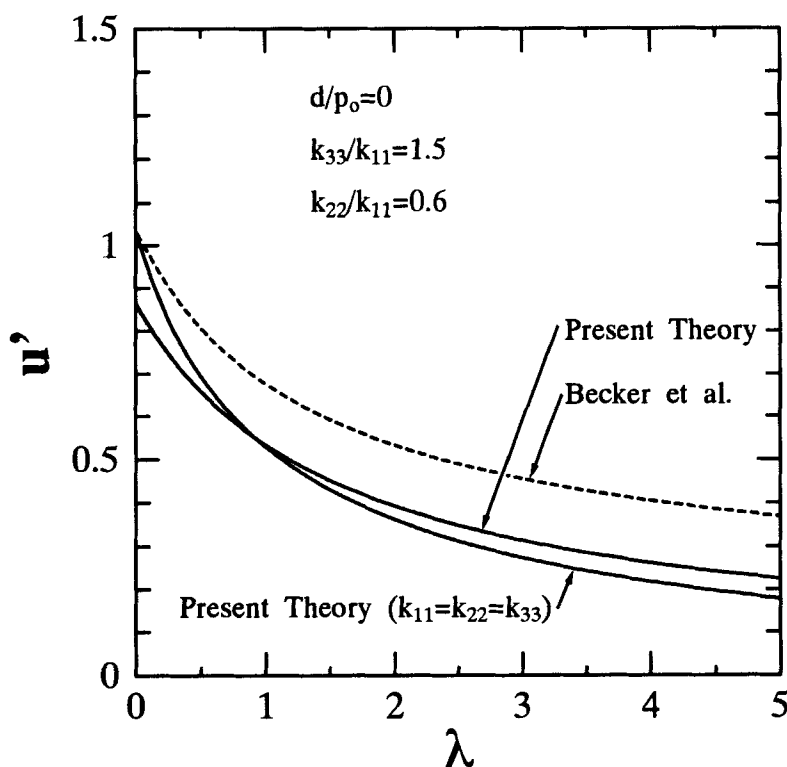


FIGURE 1 λ dependence of the reduced threshold and saturation fields of a 90° twisted slab. Solid lines show the present theoretical results and dashed lines show those reported in Ref. [9]. Material parameters used in the computation are $k_{33}/k_{11} = 1.5$, $k_{22}/k_{11} = 0.6$, and $d/p_o = 0$.

CONCLUSION

In keeping with the model of Rapini and Papoular, we have made a rigorous analysis of Fréedericksz transition field for a nematic liquid crystal cell with weak boundary coupling. In the derivations of threshold field, we only need to know one unified anchoring strength, A , but not two kinds of anchoring strength, i.e., the polar and azimuthal anchoring strengths. The rigorous surface torque balance equation derived in this paper can be applied to derive the saturation field, above which the LC slab becomes completely homeotropic. The detailed expressions of the saturation field will be shown in a forthcoming paper¹⁴. Using the present formulas, calculations of the director configuration for NLC cells with different surface anchoring and external field strength become much easier. This may have great significance in the development of LC display devices.

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