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ON THE SATURATION BEHAVIOUR OF TWISTED NEMATIC LIQUID CRYSTAL CELLS WITH A NONZERO PRETILT ANGLE*

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Equations are obtained for the surface tilt angle and the twist angle of the director in a twisted nematic liquid crystal cell under a high magnetic field. Under a zero pretilt angle, the two equations reduce to those obtained by Sugimura *et al.*[2,3] This fact has also been demonstrated numerically. With finite field strength and nonzero pretilt angle, no saturation transition exists.

Keywords: twisted nematic liquid crystal cell, weak anchoring, nonzero pretilt angle, saturation behaviour

PACC: 6130, 6470M

I. INTRODUCTION

For nematic liquid crystal (NLC) cells, surface forces are practically not strong enough to impose a well-defined orientation of the directors along the surface of the cell. For an untwisted NLC sample with weak anchoring surfaces, Rapini and Papoular[1] (R–P) proposed a phenomenological expression for a one-dimensional deformation of the interfacial energy per unit area:

$$F_S = (1/2)W\sin^2(\theta_0 - \theta_{\rm p}), \tag{1}$$

in which $\theta_{\rm p}$ is the pretilt angle, i.e. the tilt angle of the easy direction $\boldsymbol{e}$, θ_0 is the orientation of the director along the wall and the anchoring strength parameter W measures the ability of the director to deviate from the easy direction. For a twisted NLC sample, Eq.(1) may be extended to the general form:

$$F_S = -(1/2)W(\boldsymbol{n}\cdot\boldsymbol{e})^2. \tag{2}$$

With Eq.(2) Sugimura *et al.*[2,3] have discussed the threshold and the saturation fields for field-controlled chiral nematic layers with weak boundary coupling and Breddels *et al.*[4] have obtained an analytical expression for the optical threshold in highly twisted NLC with nonzero pretilt. In the following we will study the saturation behaviour for field-controlled twisted NLC with nonzero $\theta_{\rm p}$.

II. CELLS UNDER HIGH MAGNETIC FIELD

Consider a nematic cell with its two plates at z=0 and z=d respectively and with mirror symmetry with respect to z=$d/2$. The tilt angle of the director on either plate is θ_0. The easy direction on z=0 is given by

$$\boldsymbol{e} = (\cos\theta_{\rm p}, 0, \sin\theta_{\rm p}), \tag{3}$$

and the director $\boldsymbol{n}$ on plane z is given by

$$\boldsymbol{n} = [\cos\theta(z)\cos\phi(z), \cos\theta(z)\sin\phi(z), \sin\theta(z)], \tag{4}$$

where $\phi(z)$ is the angle of twist of the director on plane z. According to Eq.(2), the surface energy density on z=0 is given by

$$F_S(0) = -(1/2)W(\cos\theta_{\rm p}\cos\theta_0\cos\phi_0 + \sin\theta_{\rm p}\sin\theta_0)^2. \tag{5}$$

Under an applied magnetic field $\boldsymbol{H} = (0, 0, H)$, the free energy density of the bulk is given by

$$\begin{aligned} F_b =& (1/2)[k_{11}(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2 + k_{22}(\boldsymbol{n}\cdot\boldsymbol{\nabla}\times\boldsymbol{n})^2 \\ &+ k_{33}(\boldsymbol{n}\times\boldsymbol{\nabla}\times\boldsymbol{n})^2 - \chi_a(\boldsymbol{n}\cdot\boldsymbol{H})^2] \\ =& (1/2)[f(\theta)(\mathrm{d}\theta/\mathrm{d}z)^2 + h(\theta)(\mathrm{d}\phi/\mathrm{d}z)^2 \\ &- \chi_a H^2\sin^2\theta], \end{aligned} \tag{6}$$

where

$$f(\theta) = k_{11}\cos^2\theta + k_{33}\sin^2\theta, \tag{7}$$

$$h(\theta) = \cos^2\theta(k_{22}\cos^2\theta + k_{33}\sin^2\theta), \tag{8}$$

and k_{11}, k_{22}, k_{33}, χ_a are the splay, twist and bend elastic constants and the anisotropy of diamagnetic susceptibility, respectively.

The total free energy per unit area of the cell is now given by

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$$F = \int_0^d f_b \mathrm{d}z + 2F_S(0). \tag{9}$$

For any given field, the free energy of those cells with a stable director configuration are at their minimum. The variational calculation[5] of the total free energy gives the following equations for the equilibrium configuration of the director in the cell:

$$h(\theta)\mathrm{d}\phi/\mathrm{d}z = C_1, \tag{10}$$

$$f(\theta)(\mathrm{d}\theta/\mathrm{d}z)^2 + h(\theta)(\mathrm{d}\phi/\mathrm{d}z)^2 + \chi_a H^2 \sin^2\theta = C_2, \tag{11}$$

$$\begin{aligned} f(\theta)\mathrm{d}\theta/\mathrm{d}z|_{z=0} =& W(\cos\theta_\mathrm{p}\cos\theta\cos\phi + \sin\theta_\mathrm{p}\sin\theta) \\ & \cdot(\cos\theta_\mathrm{p}\sin\theta\cos\phi - \sin\theta_\mathrm{p}\cos\theta), \end{aligned} \tag{12}$$

$$\begin{aligned} h(\theta)\mathrm{d}\phi/\mathrm{d}z|_{z=0} =& W(\cos\theta_\mathrm{p}\cos\theta\cos\phi + \sin\theta_\mathrm{p}\sin\theta) \\ & \cdot\cos\theta_\mathrm{p}\cos\theta\sin\phi, \end{aligned} \tag{13}$$

where C_1 and C_2 are two constants of integration. Equations (12) and (13) describe the balance of torque of tilt and twist at z=0, respectively.

A. Tilt angle θ in the bulk

In case of

$$\begin{aligned} &\theta(d/2) = \theta_\mathrm{M}, \quad (\mathrm{d}\theta/\mathrm{d}z)_{z=d/2} = 0, \\ &(\mathrm{d}\phi/\mathrm{d}z)_{z=d/2} = \phi'_\mathrm{M}, \end{aligned} \tag{14}$$

Eqs.(10) and (11) lead to

$$h(\theta_\mathrm{M})\phi'_\mathrm{M} = C_1$$

and

$$h(\theta_\mathrm{M})\phi'^2_\mathrm{M} + \chi_a H^2 \sin^2\theta_\mathrm{M} = C_2, \tag{15}$$

respectively. With Eq.(15), the integration of Eq.(11) gives

$$\int_{\theta(z)}^{\theta_\mathrm{M}} N^{1/2}(\theta)\mathrm{d}\theta = (d/2) - z, \tag{16}$$

where

$$\begin{aligned} N(\theta) =& f(\theta)\{h^2(\theta_\mathrm{M})\phi'^2_\mathrm{M}[h(\theta_\mathrm{M})^{-1} - h(\theta)^{-1}] \\ & + \chi_a H^2(\sin^2\theta_\mathrm{M} - \sin^2\theta)\}^{-1}. \end{aligned} \tag{17}$$

In the range of $\pi/2 \geq \theta_\mathrm{M} \geq \theta$, let us introduce a new variable β defined by

$$\cos\theta = \cos\theta_\mathrm{M}/\cos\beta. \tag{18}$$

In terms of β, Eq.(16) becomes

$$\begin{aligned} &\int_0^{\beta(z)} \{f(\theta)/[\phi'^2_\mathrm{M}B(\theta) + \chi_a H^2](1 - \cos^2\theta_\mathrm{M}/\cos^2\beta)\}^{1/2} \\ &\cdot(\cos\beta)^{-1}\mathrm{d}\beta = (d/2) - z, \end{aligned} \tag{19}$$

where with Eqs.(7) and (8)

$$\begin{aligned} B(\theta) =& k_{33}(1 + \gamma\cos^2\theta_\mathrm{M}) \\ & \cdot[\cos^2\beta + \gamma\cos^2\theta_\mathrm{M}(1 + \cos^2\beta)] \\ & \cdot[1 + \gamma\cos^2\theta_\mathrm{M}/\cos^2\beta]^{-1}, \end{aligned}$$

and

$$\gamma = (k_{22} - k_{33})/k_{33}.$$

For the high field, in the limit of $\theta_\mathrm{M} \to \pi/2$, $B(\theta) \to k_{33}\cos^2\beta$, $f(\theta) \to k_{33}$ and Eq.(19) becomes

$$\begin{aligned} &\int_0^{\beta(z)} \{k_{33}/[k_{33}\phi'^2_\mathrm{M}\cos^2\beta + \chi_a H^2]\}^{1/2} \\ &\cdot(\cos\beta)^{-1}\mathrm{d}\beta = (d/2) - z. \end{aligned} \tag{20}$$

Evaluation of the integral[6] gives

$$\begin{aligned} &\sqrt{k_{33}/\chi_a H^2}\tanh^{-1}\{[\chi_a H^2/(k_{33}\phi'^2_\mathrm{M}\cos^2\beta \\ &+ \chi_a H^2)]^{1/2}\sin\beta\} = (d/2) - z. \end{aligned}$$

After rearrangement it becomes

$$\sin^2\beta = (1 + \xi^2\phi'^2_\mathrm{M})\tanh^2 x/(1 + \xi^2\phi'^2_\mathrm{M}\tanh^2 x), \tag{21}$$

where $\xi^{-1} = \sqrt{\chi_a H^2/k_{33}}$ and $x = (d/2 - z)/\xi$. With Eq.(18), Eq.(21) becomes

$$\cos^2\theta = \cos^2\theta_\mathrm{M}(1 + \xi^2\phi'^2_\mathrm{M}\tanh^2 x)/(1 - \tanh^2 x). \tag{22}$$

Equation (22) gives the tilt angle θ as a function of z under high fields.

B. Relationship between ϕ'_M and ϕ_0 under high field

Equations (10), (11) and (15) lead to

$$[h(\theta_\mathrm{M})\phi'_\mathrm{M}/h(\theta)]N^{1/2}(\theta)\mathrm{d}\theta = \mathrm{d}\phi. \tag{23}$$

On account of the symmetry with respect to z=$d/2$, the angle of twist $\phi(d/2)$ at the central plane of the cell is just half of the total angle of twist ϕ_t from z=0 to $z = d$. Integration of Eq.(23) leads to

$$\begin{aligned} &\int_{\theta_0}^{\theta_\mathrm{M}} h(\theta_\mathrm{M})h^{-1}(\theta)\phi'_\mathrm{M}N^{1/2}(\theta)\mathrm{d}\theta \\ &= \int_{\phi_0}^{\phi(d/2)} \mathrm{d}\phi = (\phi_t/2) - \phi_0. \end{aligned} \tag{24}$$

In the limit of $\theta_{\rm M} \to \pi/2$, Eq.(24) leads to

$$\sin^{-1}\left[\sqrt{k_{33}}\phi'_{\rm M}\sin\beta_0 \Big/ \sqrt{\chi_a H^2 + k_{33}\ \phi'^2_{\rm M}}\ \right] = (\phi_t/2) - \phi_0. \quad (25)$$

At z=0, Eq.(21) becomes

$$\sin^2\beta_0 = (1+\xi^2\phi'^2_{\rm M})\tanh^2(d/2\xi) / [1+\xi^2\phi'^2_{\rm M}\tanh^2(d/2\xi)]. \quad (26)$$

The elimination of β_0 in Eqs.(25) and (26) gives a relationship between $\phi'_{\rm M}$ and ϕ_0 in the case of a high field:

$$\phi'_{\rm M} = \tan(\phi_t/2 - \phi_0)/\xi\tanh(d/2\xi). \quad (27)$$

C. Surface tilt angle θ_0 and twist angle ϕ_0

With Eqs.(6) and (11), the total free energy Eq.(9) becomes

$$F = (C_2 - 2\chi_a H^2)(d/2) + 2\chi_a H^2 \int_0^{d/2} \cos^2\theta {\rm d}z + 2F_S(0). \quad (28)$$

With Eq.(22), Eq.(28) becomes

$$F = (C_2 - 2\chi_a H^2)(d/2) + (1/2)\chi_a H^2\cos^2\theta_{\rm M} \cdot [\xi(1+\xi^2\phi'^2_{\rm M})\sinh(d/\xi) + d(1-\xi^2\phi'^2_{\rm M})] + 2F_S(0). \quad (29)$$

At z=0, Eq.(22) becomes

$$\cos^2\theta_{\rm M} = \cos^2\theta_0[1-\tanh^2(d/2\xi)] / [1+\xi^2\phi'^2_{\rm M}\tanh^2(d/2\xi)]. \quad (30)$$

With Eqs.(15), (27) and (30), the total free energy Eq.(29) as a function of θ_0 and ϕ_0 is given by

$$\begin{aligned} F = &-(1/2)d\chi_a H^2 + \xi\chi_a H^2\tanh(d/2\xi)\cos^2\theta_0 \\ &+ 2\xi\chi_a H^2\sin^2(\phi_t/2-\phi_0)\cos^2\theta_0/\sinh(d/\xi) \\ &+ d\chi_a H^2\gamma\sin^2(\phi_t - 2\phi_0) \\ &\cdot\cos^4\theta_0/2\sinh^2(d/\xi) + 2F_s(0). \end{aligned} \quad (31)$$

In the case of $\theta_{\rm M} \to \pi/2$, with Eq.(5), up to the second order, the expansion of F in terms of $\pi/2 - \theta_0$ is given by

$$\begin{aligned} F = &-(1/2)d\chi_a H^2 - W\sin^2\theta_{\rm p} \\ &- W\sin(2\theta_{\rm p})\cos\phi_0(\pi/2-\theta_0) \\ &+ [\xi\chi_a H^2\tanh(d/2\xi) \\ &+ 2\xi\chi_a H^2\sin^2(\phi_t/2-\phi_0)/\sinh(d/\xi) \\ &- W(\cos^2\theta_{\rm p}\cos^2\phi_0 - \sin^2\theta_{\rm p})](\pi/2-\theta_0)^2. \end{aligned} \quad (32)$$

Minimization of F requires that

$$\partial F/\partial\theta_0 = 0 \quad \text{and} \quad \partial F/\partial\phi_0 = 0. \quad (33)$$

Therefore the equilibrium conditions are

$$\begin{aligned} &W\sin(2\theta_{\rm p})\cos\phi_0 - 2[\xi\chi_a H^2\tanh(d/2\xi) \\ &+ 2\xi\chi_a H^2\sin^2(\phi_t/2-\phi_0)/\sinh(d/\xi) \\ &- W(\cos^2\theta_{\rm p}\cos^2\phi_0 - \sin^2\theta_{\rm p})](\pi/2-\theta_0) = 0, \end{aligned} \quad (34)$$

and

$$\begin{aligned} &W\sin(2\theta_{\rm p})\sin\phi_0 + [W\cos^2\theta_{\rm p}\sin(2\phi_0) - 2\xi\chi_a H^2 \\ &\cdot\sin(\phi_t - 2\phi_0)/\sinh(d/\xi)](\pi/2-\theta_0) = 0. \end{aligned} \quad (35)$$

Equations (34) and (35) together determine the tilt angle θ_0 and the twist angle ϕ_0 on the surface for a high field. In the case of $\theta_{\rm p}$=0, no linear term of θ_0 appears in Eq.(32) and the anchoring energy has its extreme value at $\theta_0 = \pi/2$.

D. The case of $\theta_{\rm p}$=0

In the case of $\theta_{\rm p}$=0, Eqs.(34) and (35) reduce to

$$\begin{aligned} &\xi\chi_a H^2\tanh(d/2\xi) + 2\xi\chi_a H^2 \\ &\cdot\sin^2(\phi_t/2-\phi_0)/\sinh(d/\xi) = W\cos^2\phi_0, \end{aligned} \quad (36)$$

and

$$\xi\chi_a H^2\sin(\phi_t - 2\phi_0)/\sinh(d/\xi) = W\sin\phi_0\cos\phi_0, \quad (37)$$

respectively. Elimination of $\xi\chi_a H^2$ between Eqs.(36) and (37) gives

$$\tan\phi_0 = \sin\phi_t/2[\sinh^2(d/2\xi) + \cos^2(\phi_t/2)]. \quad (38)$$

With careful manipulation, the elimination of ϕ_0 between Eqs.(36) and (37) gives

$$\xi\chi_a H^2/W = \tanh(d/2\xi) + 2\cos^2(\phi_t/2)\sinh(d/\xi). \quad (39)$$

For an untwisted nematic slab ($\phi_t = 0$), let us introduce a dimensionless coupling parameter

$$\lambda = \pi k_{11}/Wd. \quad (40)$$

Then Eqs.(38) and (39) are simply Eqs.(57) and (56) obtained by Sugimura *et al.* in Ref.[3] respectively in the case of k_2=0 and $p_0 \to \infty$, i.e. in the case of twisted nematic cells.

Ⅲ. NUMERICAL DEMONSTRATION

In the case of $\theta_p \neq 0$ and in terms of λ, Eqs.(34) and (35) take the following forms respectively:

$$(1/\lambda)\sin(2\theta_p)\cos\phi_0 - 2[h\sqrt{k_{33}/k_{11}}\tanh\left(\pi h\sqrt{k_{11}/k_{33}}/2\right) + 2h\sqrt{k_{33}/k_{11}}\sin^2(\phi_t/2-\phi_0)/\sinh\left(\pi h\sqrt{k_{11}/k_{33}}\right) - (1/\lambda)(\cos^2\theta_p\cos^2\phi_0 - \sin^2\theta_p)](\pi/2-\theta_0) = 0, \quad (41)$$

$$(1/\lambda)\sin(2\theta_p)\sin\phi_0 + \left[(1/\lambda)\cos^2\theta_p\sin(2\phi_0) - 2h\sqrt{k_{33}/k_{11}}\sin(\phi_t-2\phi_0) / \sinh\left(\pi h\sqrt{k_{11}/k_{33}}\right)\right](\pi/2-\theta_0) = 0, \quad (42)$$

where the reduced magnetic field strength h is defined by

$$h = H/H_c, H_c = \sqrt{k_{11}/\chi_a}\ (\pi/d). \quad (43)$$

The surface tilt angle θ_0 and the twist angle ϕ_0 are now taken as functions of h.

For k_{33}/k_{11}=1.5, $\phi_t = \pi/2$ and $\theta_p = 5°$, numerical calculations show that with the increasing applied field strength, ϕ_0 approaches zero and θ_0 approaches $\pi/2$ but is not equal to $\pi/2$, as shown in Figs.1 and 2 respectively. In Figs.1 and 2, θ_0 and ϕ_0 are the surface tilt angle and the surface twist angle respectively and h is the reduced magnetic field strength. The curves A, B, C and D represent the parameters λ=0.5, 1.0, 2.0 and 5.0, respectively. The fact that the tilt angle θ_0 will not reach $\pi/2$ implies that the saturation transition cannot be defined sharply.

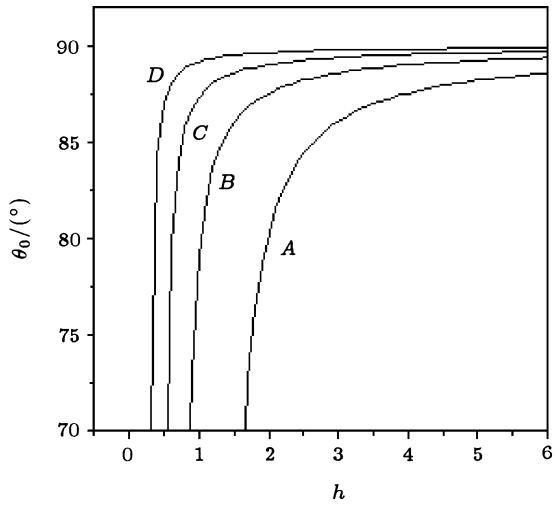


Fig.1. Surface tilt angle θ_0 as a function of reduced magnetic field strength h, predicted by the analytical result. k_{33}/k_{11}=1.5, ϕ_t=1.5, $\phi_t = \pi/2$ and $\theta_p = 5°$. Curves A, B, C and D represent the coupling parameters λ=0.5, 1.0, 2.0 and 5.0, respectively.

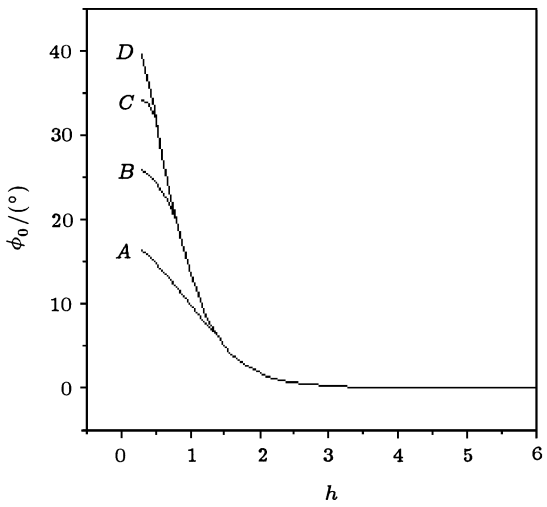


Fig.2. Surface twist angle ϕ_0 as a function of reduced magnetic field strength h, predicted by the analytical result. k_{33}/k_{11}=1.5, $\phi_t = \pi/2$ and $\theta_p = 5°$. Curves A, B, C and D represent the coupling parameters λ=0.5, 1.0, 2.0 and 5.0, respectively.

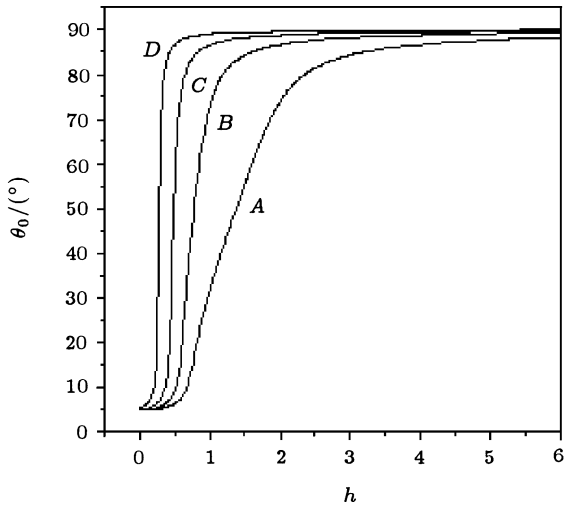


Fig.3. Surface tilt angle θ_0 as a function of reduced magnetic field strength h, predicted by the pure numerical method. k_{22}/k_{11}=0.6 k_{33}/k_{11}=1.5, $\phi_t = \pi/2$ and $\theta_p = 5°$. Curves A, B, C and D represent the coupling parameters λ=0.5, 1.0, 2.0 and 5.0, respectively.

Numerical calculations with the relaxation method[7,8] for Eqs.(10)–(13) have also been carried out under k_{22}/k_{11}=0.6, k_{33}/k_{11}=1.5, $\phi_t = \pi/2$ and $\theta_p = 5°$. These are shown in Figs.3 and 4. As in Figs.1 and 2, the curves A, B, C and D represent the parameters λ=0.5, 1.0, 2.0 and 5.0, respectively. These confirm the conclusion that no saturation transition exists for $\theta_p \neq 0$ and demonstrate even quantitatively the results of Eqs.(40) and (41) for high fields.

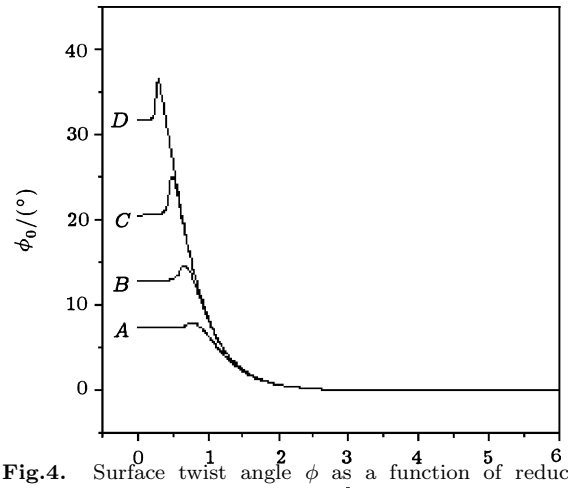


Fig.4. Surface twist angle ϕ as a function of reduced magnetic field strength h, predicted by the pure numerical method. k_{33}/k_{11}=0.6 k_{33}/k_{11}=1.5, $\phi_t = \pi/2$ and $\theta_{\rm p} = 5°$. Curves A, B, C and D represent the coupling parameters λ=0.5, 1.0, 2.0 and 5.0, respectively.

In conclusion, we have studied the saturation behaviour for field-controlled twisted NLC with a nonzero pretilt angle. Two equations are derived to determine the surface tilt angle and the twist angle of the director for high fields. These two equations can recover the saturation field obtained by Sugimura *et al.* when the pretilt angle is zero and they have been demonstrated by the direct numerical method. It has been found that there is no saturation transition at a finite field when the pretilt angle is nonzero.

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References

[1] Rapini A and Papoular M 1969 *J. Physique Coll.* **30** C4-54

[2] Sugimura A and Ou-Yang Z C 1995 *Phys. Rev.* E **51** 784

[3] Sugimura A, Luckhurst G R and Ou-Yang Z C 1995 *Phys. Rev.* E **52** 681

[4] Breddels P A and Van Sprang H A 1985 *J. Appl. Phys.* **58** 2162

[5] Jeffreys H and Jeffreys B S 1950 *Methods of Mathematical Physics* (Cambridge: Cambridge University Press) p 318

[6] Pieoce B O 1929 *A Short Table of Integrals* 3rd edn (New York: Ginn and Co) No 229

[7] Press W H, Flannery B P, Teukolsky S A and Vetterling W T 1988 *Numerical Recipes* (Cambridge: Cambridge University Press) ch 16

[8] Zhang Z D, Liu J W and Ma H M 2000 *Chin. J. Comput. Phys.* **17** 39 (in Chinese)