Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713926090

The formula of anchoring energy for a nematic liquid crystal

Yang Guo-Chen Corresponding author[a]; Zhang Shu-Jing[a]; Han Li-Jun[b]; Guan Rong-Hua[ac]
[a] Physics Institute of Hebei University of Technology, Tianjin 300130, PR China [b] Physics Department, Langfang Teachers College, Langfang Hebei 06500, PR China [c] Department of Applied Physics, North China Electric Power University, Baoding 071003, PR China

Online publication date: 12 May 2010

To cite this Article Guo-Chen Corresponding author, Yang , Shu-Jing, Zhang , Li-Jun, Han and Rong-Hua, Guan(2004) 'The formula of anchoring energy for a nematic liquid crystal', Liquid Crystals, 31: 8, 1093 — 1100
To link to this Article: DOI: 10.1080/02678290410001712541
URL: http://dx.doi.org/10.1080/02678290410001712541

LIQUID CRYSTALS, VOL. 31, NO. 8, AUGUST 2004, 1093–1100

The formula of anchoring energy for a nematic liquid crystal

YANG GUO-CHEN†*, ZHANG SHU-JING†, HAN LI-JUN‡ and GUAN RONG-HUA†§

†Physics Institute of Hebei University of Technology, Tianjin 300130, PR China
‡Physics Department, Langfang Teachers College, Langfang Hebei 06500, PR China
§Department of Applied Physics, North China Electric Power University, Baoding 071003, PR China

(*Received 26 November 2003; in final form 29 February 2004; accepted 8 March 2004*)

The interface energy for a nematic liquid crystal (NLC) is considered as the sum of potential energy between LC molecules and molecules of the substrate surface, and a formula for anchoring energy is derived by elementary principles. The anchoring energy for a NLC should have two terms, the first term is the same as the Rapini–Papoular expression, the second is related to the normal of interface and resultes from the biaxial property of a NLC induced by interface. Hence there are two anchoring coefficients, W_1 and W_2. We demonstrate that W_1 is equal to the tilt angle strength A_θ, and W_2 corresponds to the difference between A_θ and the azimuthal strength A_φ. Thus A_θ–A_φ is due to the biaxial property of the NLC near the interface. Applying this formula to the twisted NLC cell, we discuss the threshold and saturation field, as well as the maximal tilt angel θ_m with respect to A_θ/A_φ. Previously proposed formulae are discussed from our point view.

1. Introduction

It is well known that the texture of a nematic liquid crystal (NLC) layer is influenced by the interface as well as by the external field, and the distribution of the director **n** is sensitive to the interface [1]. Rapini and Papoular (RP) have introduced a simple phenomenological expression for the interfacial energy per unit area [2]: $g_s = 1/2\,A \sin^2\alpha$, where α is the angle between the director on the surface $\mathbf{n}_0$ and the easy direction **e**, and the constant A is termed anchoring strength or anchoring energy. Using the RP expression, much experimental and theoretical work has been carried out for the one-dimensional case [3–17]. The tilt anchoring strength A_θ and the azimuthal anchoring strength A_φ have also been measured. From much experiment data [18], it appears that the values of A_θ and A_φ are different (commonly, $A_\theta \gg A_\varphi$ [1]).

When two-dimensional cases (such as a twisted NLC cell) are considered, a general anchoring energy expression is necessary. Two modes generalize the RP expression using the phenomenological method. The first is a single-parameter formula, expressed by [17]

$$g_s = -1/2A(\mathbf{n}\cdot\mathbf{e})^2. \tag{1}$$

The second is a two-parameter formula expressed by [9–16]

$$g_s = 1/2A_\theta \sin^2\left(\theta^0 - \theta_0\right) + 1/2A_\varphi \sin^2\left(\varphi^0 - \varphi_0\right) \tag{2}$$

in which appear two anchoring strength parameters. Becia *et al.* [19] have made a meaningful improvement to equation (2), but their expression is still incomplete, and gives wrong predictions for the homeotropic anchoring case.

More recently, Zhao *et al.* [20–22] have proposed a two-parameter and one easy director expression through a second order spherical-harmonic expansion of the anchoring energy, which can be expressed by

$$g_s = W_\zeta(\mathbf{n}\cdot\boldsymbol{\xi})^2 + W_\eta(\mathbf{n}\cdot\boldsymbol{\eta})^2 \tag{3}$$

where the unit vector $\boldsymbol{\xi}$, $\boldsymbol{\eta}$, together the easy axis $\boldsymbol{\varepsilon}$, are the stationary directions of the second order anchoring energy.

Recently the voltage-controlled twist (VCT) effect [23] has attracted attention. This effect appears in a liquid crystal film with negative dielectric anisotropy sandwiched between a homeotropic substrate with in-plane grooving and a unidirectional planar anchoring surface. Various authors have explained this effect from different phenomenological views. Bryan-Brown *et al.* [23] postulated that a grooving homeotropic substrate has two easy directions. However Zhao *et al.* [20, 21] explained the effect with one easy direction but two anchoring strength parameters.

In considering the various phenomenological

*Author for correspondence; e-mail: Yang_gc@hotmail.com

Liquid Crystals ISSN 0267-8292 print/ISSN 1366-5855 online © 2004 Taylor & Francis Ltd
http://www.tandf.co.uk/journals
DOI: 10.1080/02678290410001712541

expressions described above, there is a great need for a theoretical formula derived by elementary principles to analyse these expressions, and to improve them. This theory should answer (i) why A_θ is different from A_φ; (ii) the physical mechanism for one easy director or two easy directors, (iii) the physical reason for one anchoring strength or two strength parameters.

In this paper, we attempt to derive the formula for anchoring energy by elementary principles. Consider that the interface energy is the sum of interactional potential energy between LC molecules and the molecules of the substrate surface in principle, and the anchoring energy is the anisotropic part of this energy. By supposing a possible form of this potential, we obtain

$$g_s = -\frac{1}{2} W_1 (\mathbf{n}\cdot\mathbf{e})^2 - \frac{1}{2} W_2 (\mathbf{n}\cdot\mathbf{e}\times\mathbf{v})^2 \tag{4}$$

where $\mathbf{n}$ and $\mathbf{v}$ are the directors of the LC and the normal of the interface, respectively, and $\mathbf{e}$ is the average orientation or equivalent orientation of molecules of substrate the surface. Both W_1 and W_2 are related to potential. In addition W_1 is approximately proportional to the scalar order parameter S, and W_2 is related to the biaxial property of the NLC near the interface.

Comparing our expression with the RP expression for the one-dimension case, we obtain

$$A_\theta = W_1, \quad A_\varphi = W_1 - W_2 \tag{5}$$

This means that $A_\theta - A_\varphi$ is due to the biaxial property of the NLC near the interface.

With expression (4) we investigate the weak anchoring twisted NLC cell, and calculate the threshold field and saturation field, and examine the effect of the biaxial property, i.e. the difference between A_θ and A_φ. We also discuss the relationship between the maximum tilt angle θ_m and external field h for different values of A_θ/A_φ Comparing our result with reference [17], we see that the effect of the biaxial property is important, especially for values of the saturated field h_{sat} and the maximum tilt angle θ_m.

We follow by discussing some phenomenological expressions, including the formula proposed in [20], and give a conclusion.

2. Microcosmic theory of anchoring energy

The anchoring energy is the anisotropic part of the interface energy and can be seen as the anisotropic part of the sum of interaction potentials between LC molecules and molecules of the substrate surface, in principle. Suppose molecules of the substrate surface have an orientation or equivalent orientation $\mathbf{e}$, then the anistropic part of potential between the ith LC molecule with τth molecule of the substrate surface can be expressed as

$$V_{i,\tau} = V(|\mathbf{r}_i - \mathbf{R}_\tau|)(\boldsymbol{\Omega}_i\cdot\mathbf{e}_\tau)^2 \tag{6}$$

where $\mathbf{r}_i$ is the position vector of the centroid of the liquid crystal molecule, and $\mathbf{R}_\tau$ is the position vector of the centroid of the substrate surface molecule, $\boldsymbol{\Omega}_i$ and $\mathbf{e}_\tau$ are their orientations, respectively. Then the anchoring energy can be expressed as

$$g_s = \sum_{i,\tau}{}' V_{i,\tau} \tag{7}$$

For simplification, we suppose that all molecules of the substrate surface have the same orientation $\mathbf{e}$ on average, and $V(|\mathbf{r}_i - \mathbf{R}_\tau|)$ is constant. If $V(|\mathbf{r}_i - \mathbf{R}_\tau|)$ is negative, it can be denoted by $-V$ ($V>0$). Otherwise, when $V(|\mathbf{r}_i - \mathbf{R}_\tau|)$ is positive it should be denoted by V. Suppose $V(|\mathbf{r}_i - \mathbf{R}_\tau|)$ is negative temporarily; adopt the nearest neighbour interaction approximation and put the number of terms in summation of equation (7) as N, then

$$g_s = -NV\langle(\boldsymbol{\Omega}\cdot\mathbf{e})^2\rangle \tag{8}$$

where $\langle\ldots\rangle$ donates the statistical average.

It is well known that the order parameter tensor $\mathbf{Q}_{\mu\nu}$ is given by

$$\mathbf{Q}_{\mu\nu} = \frac{3}{2}\boldsymbol{\Omega}_\mu\boldsymbol{\Omega}_\nu - \frac{1}{2}\delta_{\mu\nu} \tag{9}$$

Since $\mathbf{Q}_{\mu\nu}$ is symmetric it can be diagonalized by choosing the appropriate coordinate frame. The diagonal form can be written as

$$\mathbf{Q} = \begin{pmatrix} -\frac{1}{2}S - P & 0 & 0 \\ 0 & -\frac{1}{2}S + P & 0 \\ 0 & 0 & S \end{pmatrix} \tag{10}$$

where S is the uniaxial order parameter.

$$S = \frac{3}{2}\langle\boldsymbol{\Omega}_z^2\rangle - \frac{1}{2} \tag{11}$$

and

$$P = \frac{3}{4}\langle(\boldsymbol{\Omega}_y^2 - \boldsymbol{\Omega}_x^2)\rangle \tag{12}$$

is the biaxial parameter. Whereas for LCs in the bulk P is equal to zero because nematics are uniaxial; close to interfaces P may become finite because the interface breaks the symmetry. The values of P have been investigated experimentally [24–26]. We consider that the biaxial property of a NLC near the substrate is an important physical condition.

We now calculate the statistical average in equation (8) by using equation (10). Consider an interface between the liquid crystal and substrate surface shown in figure 1. The normal of the interface is $\mathbf{v}$ and the

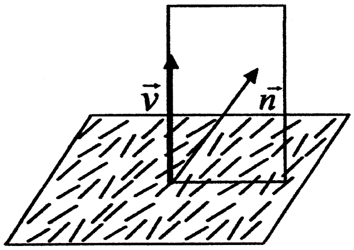

Figure 1. Schematic of interface of LC with the substrate; **v** is the normal to the interface, **n** is the director of the LC.

director of the LC is **n**. If **n** is not parallel to the **v**, then the C_∞ symmetry of the LC is broken. However, the symmetry respective to the plane defined by **n** and **v** persists, as shown figure 1.

We can now adopt the proper coordinate system in which the order parameter tensor **Q** can be expressed by equation (10), such as in the case of liquid crystal S_c [27]. The unit vectors of the three coordinate axes can be written as

$$\hat{z}=\mathbf{n},\quad \hat{y}=\frac{\mathbf{v}\times\mathbf{n}}{|\mathbf{v}\times\mathbf{n}|},\quad \hat{x}=\frac{(\mathbf{v}\times\mathbf{n})\times\mathbf{n}}{|\mathbf{v}\times\mathbf{n}|}. \tag{13}$$

Then from equation (9) have

$$\begin{aligned}\langle\boldsymbol{\Omega}_1^2\rangle&=\frac{1}{3}(1-S)-\frac{2}{3}P\\ \langle\boldsymbol{\Omega}_2^2\rangle&=\frac{1}{3}(1-S)+\frac{2}{3}P\\ \langle\boldsymbol{\Omega}_3^2\rangle&=\frac{1}{3}(1+2S)\end{aligned} \tag{14}$$

and

$$\langle\boldsymbol{\Omega}_\mu\boldsymbol{\Omega}_v\rangle=0,\quad \text{for } \mu\neq v \tag{15}$$

Substitution equation (14) into equation (8) yields

$$g_s=-NV\left\{\langle\boldsymbol{\Omega}_1^2\rangle e_1^2+\langle\boldsymbol{\Omega}_2^2\rangle e_2^2+\langle\boldsymbol{\Omega}_3^2\rangle e_3^2\right\} \tag{16}$$

where we put $\mathbf{e}=(e_1,e_2,e_3)$. By using equation (13)

$$e_1^2=1-e_2^2-e_3^2,\quad e_2=\mathbf{e}\cdot\frac{\mathbf{v}\times\mathbf{n}}{|\mathbf{v}\times\mathbf{n}|},\quad e_3=\mathbf{e}\cdot\mathbf{n}$$

and from equation (8), we obtain

$$\begin{aligned}g_s=&-NV\left(S+\frac{2}{3}P\right)(\mathbf{n}\cdot\mathbf{e})^2-\frac{4}{3}NV\frac{P}{|\mathbf{v}\times\mathbf{n}|^2}(\mathbf{n}\cdot\mathbf{e}\times\mathbf{v})^2\\ &-\frac{1}{3}NV[(1-S)+2P]\end{aligned} \tag{17}$$

The last term in equation (17) is a constant. We see thant g_s is related to the biaxial parameter P. If the value of P is small, then (17) can be re-expressed approximately by

$$g_s=-NVS(\mathbf{n}\cdot\mathbf{e})^2-\frac{4}{3}NV\frac{P}{|\mathbf{v}\times\mathbf{n}|^2}(\mathbf{n}\cdot\mathbf{e}\times\mathbf{v})^2 \tag{18}$$

Put

$$W_1=2NVS \tag{19}$$

$$W_2=\frac{8}{3}NV\frac{P}{|\mathbf{v}\times\mathbf{n}|^2} \tag{20}$$

then $g_s=-\frac{1}{2}W_1(\mathbf{n}\cdot\mathbf{e})^2-\frac{1}{2}W_2(\mathbf{n}\cdot\mathbf{e}\times\mathbf{v})^2$.
This is equation (4). Note here we suppose $V(|\mathbf{r}_i-\mathbf{R}_\tau|)$ is negative.

Two points arise from the foregoing:

(i) The formulae show that the anchoring energy g_s has two easy directors $\mathbf{n}=\mathbf{e}$ and $\mathbf{n}=\mathbf{e}\times\mathbf{v}$ (see the Appendix for more details). The latter is due to the biaxial property induced by the interface.
(ii) There are two strength parameters W_1 and W_2. Both are proportional to the potential strength V. Furthermore, W_1 is proportional to the scalar order parameter S and W_2 is related to the biaxial parameter P. Obviously, P is relevant to the tilt angle θ of **n**. For example, when $\theta=\pi/2$, C_∞ persists, and $P=0$; however when $\theta=0$, the value of P is maximum. P is therefore a function of θ; only when P is small and proportional to $\cos^2\theta$, are W_1 and W_2 constant. Otherwise, the formula should be modified†.

Suppose both W_1 and W_2 are constant. They should be related to A_θ and A_τ. Putting

$$\begin{aligned}\mathbf{e}&=(\cos\Theta\cos\Phi,\Theta\sin\Phi,\sin\Theta)\\ \mathbf{n}&=(\cos\theta\cos\varphi,\cos\theta\sin\varphi,\sin\theta)\\ \mathbf{v}&=(0,0,1)\end{aligned} \tag{21}$$

then

$$\begin{aligned}g_s=&-\frac{1}{2}W_1[\cos\theta\cos\Theta\cos(\varphi-\Phi)+\sin\theta\sin\Theta]^2\\ &-\frac{1}{2}W_2[\cos\theta\cos\Theta\sin(\varphi-\Phi).\end{aligned} \tag{22}$$

For the one-dimensional case, if $\varphi=\Phi$, we obtain $W_1=A_\theta$ and if $\theta=\Theta$ equation (22) yields $g_s=-1/2(W_1-W_2)\cos^2(\varphi-\Phi)-1/2W_1$, giving $A_\varphi=W_1-W_2$. This means that the difference between A_θ and A_φ is due to the biaxial property of the NLC near the interface.

Formula (4) is a theoretical result. We know that there may be some doubts in the derivation; for example, the expression of interaction potential between LC molecules and molecules of the substrate

†If P is not small enough, then $W_1=2NV(S+\frac{2}{3}P)$. P is function of tilt angle θ of **n**, it can be expressed by $P=\delta_1\cos^2\theta+\delta_2\cos^4\theta+\ldots\approx\delta_1\cos^2\theta$ by considering invariance of $\mathbf{n}=-\mathbf{n}$ and for $\theta=\frac{\pi}{2}$, $P=0$. Then for one-dimensional planar anchoring $g=\frac{1}{2}A_1\sin^2\theta+\frac{1}{2}A_2\sin^4\theta$.

surface, the biaxial property of a NLC near the interface, and the supposition that W_1 and W_2 are constants, etc. However, this theory is a correct approach and the its validity can be examined by experimental result. In a later section we discuss the twisted NLC cell, using equation (4).

3. The twisted NLC cell and chiral NLC cell

In order to examine the effect of the biaxial property induced by the interface, we now investigate the twisted NLC cell using anchoring energy formula (4) and compare our results with previous studies [17]. We consider a nematic cell of thickness of l located between $z=0$ and $z=l$ of a Cartesian coordinate system. We put

$$\mathbf{e}=(1, 0, 0) \quad \text{for } z=0 \tag{23}$$

$$\mathbf{e}=(\cos\varphi_t, \sin\varphi_t, 0) \quad \text{for } z=l \tag{24}$$

where φ_1 is the twist angel, e.g. $\varphi_t=0{,}90^\circ{,}270^\circ$, etc. The external magnetic field is

$$\mathbf{H}=(0, 0, H) \tag{25}$$

The director $\mathbf{n}$ may be expressed as

$$\mathbf{n}=(\cos\theta\cos\varphi, \cos\theta\sin\varphi, \sin\theta) \tag{26}$$

where θ and φ are the tilt and azithmual angles, respectively. The anchoring energies of the substrate at $z=0$ and $z=l$ are, respectively

$$g_s^- = -\frac{1}{2}W_1\cos^2\theta_0\cos^2\varphi_0 - \frac{1}{2}W_2\cos^2\theta_0\sin^2\varphi_0 \quad \text{for } z=0 \tag{27}$$

$$g_s^+ = -\frac{1}{2}W_1\cos^2\theta_l\cos^2(\varphi_t-\varphi_l) - \frac{1}{2}W_2\cos^2\theta_l\sin^2(\varphi_t-\varphi_l) \quad \text{for } z=l \tag{28}$$

The total free energy [27] is

$$\begin{aligned} G &= S\int_0^l g_b\mathrm{d}z + \int g_s\mathrm{d}s \\ &= S\int_0^l \left[\frac{1}{2}f(\theta)(\frac{\mathrm{d}\theta}{\mathrm{d}z})^2 + \frac{1}{2}h(\theta)(\frac{\mathrm{d}\varphi}{\mathrm{d}z})^2 + k_2\cos^2\theta\frac{\mathrm{d}\varphi}{\mathrm{d}z} + \frac{k_2^2}{2k_{22}} - \frac{1}{2}\chi_\alpha\mathbf{H}^2\sin^2\theta\right]\mathrm{d}z \\ &\quad + S\big(-W_1\cos^2\theta_0\cos^2\varphi_0 - W_2\cos^2\theta_0\sin^2\varphi_0\big) \end{aligned} \tag{29}$$

where

$$f(\theta)=k_{11}\cos^2\theta + k_{33}\sin^2\theta \tag{30}$$

$$h(\theta)=\cos^2\theta\big(k_{22}\cos^2\theta + k_{33}\sin^2\theta\big) \tag{31}$$

$$k_2 = -k_{22}\frac{2\pi}{p_0} \tag{32}$$

and k_{11}, k_{22} and k_{33} are splay, twist and bend elastic constants of the LC, respectively, p_0 denotes the pitch of the material. Applying the variation calculus of θ and φ of G [28, 29], respectively, we obtain

$$f(\theta)\theta'' + \frac{1}{2}\frac{\mathrm{d}f(\theta)}{\mathrm{d}\theta}\theta'^2 - \frac{1}{2}\frac{\mathrm{d}h(\theta)}{\mathrm{d}\theta}\varphi'^2 + 2k_2\sin\theta\cos\theta\varphi' + \chi_\alpha H^2\sin\theta\cos\theta = 0 \tag{33}$$

$$\varphi' = \frac{1}{h(\theta)}\big(C_1 - k_2\cos^2\theta\big) \tag{34}$$

where C_1 is a constant. Substitution of equation (34) into equation (33) leads to

$$f(\theta)\theta'^2 = \chi_\alpha H^2(\sin^2\theta_m - \sin^2\theta) + \frac{1}{h(\theta_m)}(C_1 - k_2\cos^2\theta_m)^2 - \frac{1}{h(\theta)}(C_1 - k_2\cos^2\theta)^2 \tag{35}$$

where $\theta_m=\theta(l/2)$ and is dependent on the applied field.

The boundary conditions for the lower substrate surface are given by

$$f(\theta_0)\frac{\mathrm{d}\theta}{\mathrm{d}z}\Big|_{z=0} = (W_1 - W_2)\sin\theta_0\cos\theta_0\cos^2\varphi_0 + W_2\sin\theta_0\cos\theta_0 \tag{36}$$

$$h(\theta_0)\frac{\mathrm{d}\varphi}{\mathrm{d}z}\Big|_{z=0} + k_2\cos^2\theta_0 = (W_1 - W_2)\cos^2\theta_0\sin\varphi_0\cos\varphi_0 \tag{37}$$

The integration of equation (35) becomes

$$\frac{l}{2} = \int_{\theta_0}^{\theta_m}(N(\theta))^{\frac{1}{2}}\mathrm{d}\theta \tag{38}$$

where $N(\theta)$ is defined by

$$N(\theta) = f(\theta)\left[\chi_\alpha H^2(\sin^2\theta_m - \sin^2\theta) + \frac{C_1 - k_2\cos^2\theta_m}{h(\theta_m)} - \frac{C_1' - k_2\cos^2\theta}{h(\theta)}\right]^{-1} \tag{39}$$

and $C_1=(W_1-W_2)\cos^2\theta\sin\varphi_0\cos\varphi_0$ can be obtained through substitution of equation (34) into (37).

Also, equation (34) can be expressed by

$$\mathrm{d}\varphi = \frac{(N(\theta))^{\frac{1}{2}}}{h(\theta)}\big(C_1 - k_2\cos^2\theta\big)\mathrm{d}\theta \tag{40}$$

and for boundary conditions equation (36) becomes

$$\frac{f(\theta_0)}{(N(\theta_0))^{\frac{1}{2}}} = (W_1 - W_2)\sin\theta_0\cos\theta_0\cos^2\varphi_0 + W_2\sin\theta_0\cos\theta_0. \qquad (41)$$

In order to discuss some problems over the whole range $(0, \infty)$ of the external field H, we make a variable transformation. Putting $u=\sin^2\theta_{\mathrm{m}}$ and adopting the new variable v to displace θ,

$$v = \frac{\tan^2\theta}{\tan^2\theta_{\mathrm{m}}},\ v_0 = \frac{\tan^2\theta_0}{\tan^2\theta_{\mathrm{m}}}. \qquad (42)$$

Meanwhile, we introduce the dimensionless parameter $\lambda = \pi k_{22}/(W_1 l)$, $\varpi = W_1/(W_1 - W_2) = A_\theta/A_\varphi$, and the reduced magnetic field $h = H/H_c^0$ (where $H_c = \pi/l(k_{11}/\chi_\alpha)^{\frac{1}{2}}$). Substituting equation (42) into equation (38), we obtain

$$\pi h = \int_{v_0}^{1}\left(\frac{1-u+uv+\gamma}{1-v}\right)^{\frac{1}{2}}\left(\frac{1}{1+X}\right)^{\frac{1}{2}}\frac{1}{v}\mathrm{d}v. \qquad (43)$$

Substitution of equation (42) into (40) and (41) gives

$$\frac{1}{2}\varphi_1 - \varphi_0 = \frac{1}{\varpi\lambda h}\int_{v_0}^{l}\left(\frac{1-u+uv+\gamma uv}{1-v}\right)^{\frac{1}{2}}\left(\frac{1}{1+X}\right)^{\frac{1}{2}} \times \frac{\sin\varphi_0\cos\varphi_0(1-u+uv) + 2\varpi\lambda l/p_0(1-u+uv_0)}{2(1-u+uv+\eta uv)(1-u+uv_0)v^{\frac{1}{2}}}\mathrm{d}v \qquad (44)$$

$$h = \frac{k_{22}}{k_{11}}\frac{1}{\varpi\lambda}\frac{(1-u+uv_0+\gamma uv_0)^{\frac{1}{2}}}{1-u+uv_0+\gamma uv_0}\frac{1}{(1+X_0)^{\frac{1}{2}}}\frac{v_0^{\frac{1}{2}}}{(1-v_0)^{\frac{1}{2}}} \times (\cos^2\varphi_0 + \varpi - 1)\mathrm{d}v \qquad (45)$$

where

$$X = (1-u+uv)\frac{k_{22}}{k_{11}}\left\{\frac{\sin^2\varphi_0\cos^2\varphi_0[(1+\eta u)(2-u+uv)-(1+\eta)]}{(\varpi\lambda)^2h^2(1-u+uv_0)^2(1+\eta u)(1-u+uv+\eta uv)} - \frac{(2\varpi\lambda l/p_0)^2(1+\eta)^2(1-u+uv_0)^2 + 4\varpi\lambda l\eta/p_0\sin\varphi_0\cos\varphi_0(1-u)(1-u+uv_0)}{(\varpi\lambda)^2h^2(1-u+uv_0)^2(1+\eta u)(1-u+uv+\eta uv)}\right\} \qquad (46)$$

and $\gamma = (k_{33} - k_{11})/k_{11}$, $\eta = (k_{33} - k_{22})/k_{22}$.

For a given value magnetic field h, the values of v_0, φ_0 and θ_{m} can be determined from equations (43)–(46).

We now discuss the threshold field H_{th}, the saturation field H_{sat} and the maximum tilt angle θ_{m}.

The threshold field H_{th}. Taking the limit $u=0$ at the point of threshold, equations (46), (43), (44) and (45) become

$$X_{\mathrm{th}} = \frac{1}{(\varpi\lambda)^2h_{\mathrm{th}}^2}\frac{k_{22}}{k_{11}}[\sin^2\varphi_0\cos^2\varphi_0(1-\eta) - (2\varpi\lambda\frac{l}{p_0})^2(1+\eta) + 4\varpi\lambda\frac{l}{p_0}\sin\varphi_0\cos\varphi_0] \qquad (47)$$

$$\frac{\pi h_{\mathrm{th}}}{2} = \int_{v_0}^{l}\frac{1}{2(v(1-v))^{\frac{1}{2}}}\frac{1}{(1+X_{\mathrm{th}})^{\frac{1}{2}}}\mathrm{d}v \qquad (48)$$

$$\frac{1}{2}\varphi_{\mathrm{t}} - \varphi_0 = \frac{\sin\varphi_0\cos\varphi_0 - 2\pi\lambda l/p_0}{\varpi\lambda} \times \int_{v_0}^{1}\frac{1}{2(v(1-v))^{\frac{1}{2}}}\frac{1}{(1+X_{\mathrm{th}})^{\frac{1}{2}}}\mathrm{d}v \qquad (49)$$

$$h_{\mathrm{th}} = \frac{k_{22}}{k_{11}}\frac{1}{\varpi\lambda}\left(\frac{1}{1+X_{\mathrm{th}}}\right)^{\frac{1}{2}}\left(\frac{v_0}{1-v_0}\right)^{\frac{1}{2}}(\varpi - \sin^2\varphi_0). \qquad (50)$$

From equation (48) and (49), we obtain

$$\varphi_1 - 2\varphi_0 = \frac{2\pi l}{p_0} + \frac{\pi}{\varpi\lambda}\sin\varphi_0\cos\varphi_0 \qquad (51)$$

and

$$\left(\frac{1-v_0}{v_0}\right)^{\frac{1}{2}} = \tan\left[\frac{\pi}{2}h_{\mathrm{th}}(1+X_{\mathrm{th}})^{\frac{1}{2}}\right]. \qquad (52)$$

Substitution of equation (48) into (50) gives

$$\varpi - \sin^2\varphi_0 = \frac{k_{11}}{k_{22}}\varpi\lambda h_{\mathrm{th}}(1+X_{\mathrm{th}})^{\frac{1}{2}}\tan\left[\frac{\pi}{2}h_{\mathrm{th}}(1+X_{\mathrm{th}})^{\frac{1}{2}}\right]. \qquad (53)$$

Note that our results are the same as in reference [17] when $\varpi = 1$, i.e. $A_\theta = A_\varphi$.

We now carry out the numerical calculations with the same material parameters as used in [17]. Figures 2 and 3 shows that λ and ϖ are dependent on the threshold field for $\varphi_{\mathrm{t}} = \pi/2$ and $\varphi_{\mathrm{t}} = 3\pi/2$. We see that for $\varphi_{\mathrm{t}} = 3\pi/2$ the value of the threshold field clearly becomes smaller with the increase of ϖ.

The saturation field H_{sat}. Taking the limit $u \to 1$, equations (46), (43), (44) and (45) become

$$X_{\mathrm{sat}} = \frac{k_{22}}{k_{11}}\frac{\sin^2\varphi_0\cos^2\varphi_0 v - (2\varpi\lambda l/p_0)^2v_0^2}{(\varpi\lambda)^2h_{\mathrm{sat}}^2(1+\eta)} \qquad (54)$$

$$\pi h_{\mathrm{sat}} = (1+\gamma)^{\frac{1}{2}}\int_{v_0}^{1}\frac{1}{v(1-v)^{\frac{1}{2}}(1+X_{\mathrm{sat}})^{\frac{1}{2}}}\mathrm{d}v \qquad (55)$$

$$\frac{1}{2}\varphi_{\mathrm{t}} - \varphi_0 = \frac{(1+\gamma)^{\frac{1}{2}}}{2\varpi\lambda h_{\mathrm{sat}}(1+\eta)v_0}\int_{v_0}^{1}\frac{\sin\varphi_0\cos\varphi_0 v + 2\varpi\lambda l/p_0 v_0}{v(1-v)^{\frac{1}{2}}(1+X_{\mathrm{sat}})^{\frac{1}{2}}}\mathrm{d}v \qquad (56)$$

Then the integration of equation (55) can be performed analytically to give

$$\tan\left(\frac{\pi Y}{2}\right) = \frac{\varpi\lambda Y(v_0(1-v_0))^{\frac{1}{2}}}{\left[(\varpi\lambda)^2Y^2v_0^2 + (k_{22}/k_{33})^2\sin^2\varphi_0\cos^2\varphi_0\right]^{\frac{1}{2}}} \qquad (57)$$

where

$$Y = \left[h_{\mathrm{sat}}^2\left(\frac{k_{11}}{k_{33}}\right) - \left(\frac{2k_{22}}{k_{33}}\frac{l}{p_0}\right)\right]^{\frac{1}{2}}. \qquad (58)$$

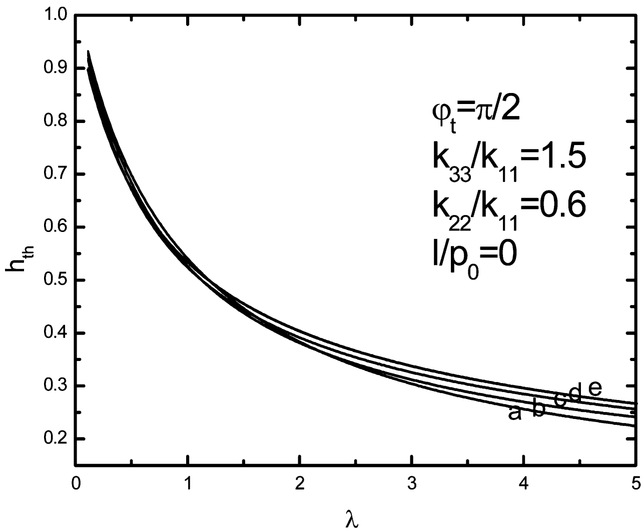

Figure 2. Dependence of the reduced threshold field h_{th} on λ and ϖ for a twisted nematic cell. a: $\varpi=1$, b: $\varpi=2$, c: $\varpi=5$, d: $\varpi=20$, e: $\varpi=50$.

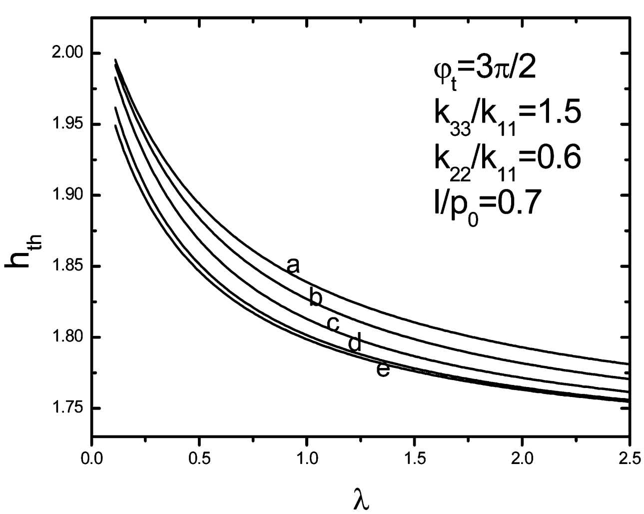

Figure 3. Dependence of the reduced threshold field h_{th} on λ and ϖ for a supertwist cell. a: $\varpi=1$, b: $\varpi=2$, c: $\varpi=5$, d: $\varpi=20$, e: $\varpi=50$.

With a similar process, the integration of equation (56) can be obtained as

$$\frac{1}{2}\varphi_{\mathrm{t}}-\varphi_0-\frac{\pi l k_{22}}{p_0 k_{33}}=$$
$$\sin^{-1}\left\{\frac{k_{22}/k_{33}\sin\varphi_0\cos\varphi_0(1-v_0)^{\frac{1}{2}}}{\left[(\varpi\lambda)^2Y^2v_0^2+(k_{22}/k_{33})^2\sin^2\varphi\cos^2\varphi_0\right]^{\frac{1}{2}}}\right\} \tag{59}$$

And the boundary condition (45) changes to

$$\varpi-\sin^2\varphi_0=$$
$$\left[(\varpi\lambda)^2Y^2v_0+(k_{22}/k_{33})^2\sin^2\varphi_0\cos^2\varphi_0\right]^{\frac{1}{2}}\frac{(1-v_0)^{\frac{1}{2}}}{v_0^{\frac{1}{2}}}. \tag{60}$$

From equations (57), (59), and (60), we obtain the relationship between λ and the reduced saturation field h_{sat}

$$\varpi\lambda\frac{k_{33}}{k_{22}}=\frac{\tanh(\pi Y/2)}{Y}\left\{1+\frac{\cos^2 T}{\sin^2(\pi Y/2)}\right.$$
$$+(\varpi-1)\left[2+\frac{1}{\sinh^2(\pi Y/2)}\right. \tag{61}$$
$$\left.\left.-\frac{1}{Y\lambda k_{33}/k_{22}\tanh(\pi Y/2)}\right]\right\}$$

where $T\equiv\varphi_{\mathrm{t}}/2-\pi l k_{22}/(p_0k_{33})$.

In Figures 4 and 5, it is clearly seen that λ and ϖ are dependent on the saturation field $\varphi_{\mathrm{t}}=\pi/2$ and $\varphi_{\mathrm{t}}=3\pi/2$ respectively. We note that the saturation field h_{sat} increases with increase of ϖ for $\varphi_{\mathrm{t}}=\pi/2$; however, it decreases with increase of ϖ for $\varphi_{\mathrm{t}}=3\pi/2$.

From above calculations, we find that the difference between A_θ and A_φ affects both the threshold and saturation fields, and is greater for the latter.

The maximum tilt angle θ_m. By using equations (33), (44) and (45), we can obtain the value of u for a given value of the external field **H** and the maximal tilt angle θ_{m} is also obtained. The results are shown in Figure 6,

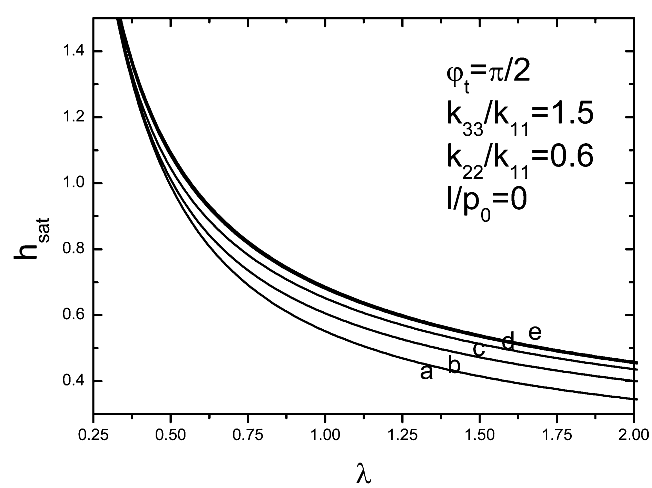

Figure 4. Dependence of the reduced saturation field h_{sat} on λ and ϖ for a twisted nematic cell. a: $\varpi=1$, b: $\varpi=2$, c: $\varpi=5$, d: $\varpi=20$, e: $\varpi=50$.

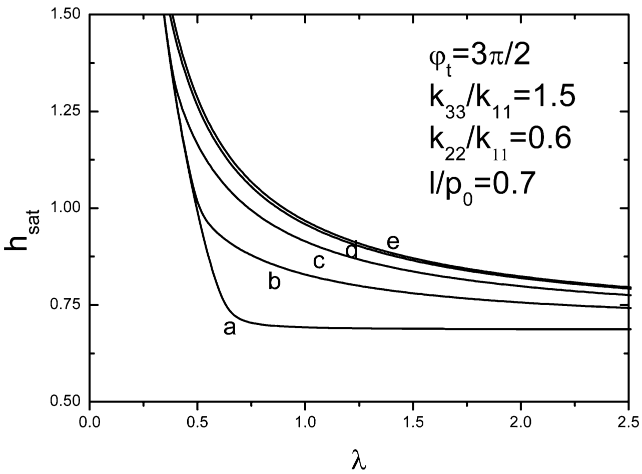

Figure 5. Dependence of the reduced saturation field h_{sat} on λ and ϖ for a supertwist cell. a: $\varpi=1$, b: $\varpi=2$, c: $\varpi=5$, d: $\varpi=20$, e: $\varpi=50$.

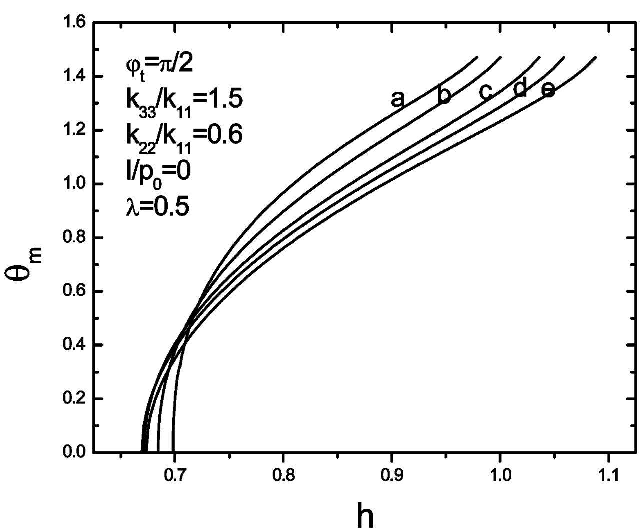

Figure 6. Dependence of the reduced saturation field h_{sat} on maximum θ_m for anchoring energy $\lambda=0.5$; a: $\varpi=1$, b: $\varpi=2$, c: $\varpi=5$, d: $\varpi=20$, e: $\varpi=50$.

which indicates that θ_m becomes smaller with increasing ϖ for $\lambda=0.5$ in high field **H**.

We note that the authors of reference [22] have calculated the threshold and saturation properties of a twisted NLC under an electric field. Their formulae for anchoring energy are discussed below.

4. Discussion and conclusion

We have deduced the formula for anchoring energy from microcosmic theory in §2 This result is based on the precondition that the anisotropic part of the interaction potential between two species of molecules $V(i,\tau)$ is negative. However, for some cases $V(i,\tau)$ is positive. For these cases, g_s should be

$$g_s=1/2W_1(\mathbf{n}\cdot\mathbf{e})^2+1/2W_2(\mathbf{n}\cdot\mathbf{e}\times\mathbf{v})^2 \tag{62}$$

where W_1 and W_2 are expressed by equations (19) and (20), and are positive. Then the minimum value of g_s occurs at $\mathbf{n}=\boldsymbol{\varepsilon}$, and $\boldsymbol{\varepsilon}$ should be perpendicular to both **e** and $\mathbf{e}\times\mathbf{v}$,

$$\boldsymbol{\varepsilon}=\mathbf{e}\times(\mathbf{e}\times\mathbf{v})/|\mathbf{e}\times\mathbf{v}|. \tag{63}$$

We now compare our expression in equation (63) with the formula proposed by Zhao *et al.* [20, 21, 22], and find that g_s is the same. Zhao *et al.* have explained the VCT effect by means of their formula.

We conclude:

(1) For common cases, $V(i,\tau)$ is negative, and two easy directions and two strength parameters appear. The orientation or equivalent orientation of substrate molecules **e** is one of the easy directions.

(2) For other cases, $V(i,\tau)$ may be positive. Then there is one easy direction and two strength parameters.

Appendix

Put $\mathbf{n}=(n_1, n_2, n_3)$, $\mathbf{e}=(e_1, e_2, e_3)$, $\mathbf{a}=\mathbf{e}\times\mathbf{v}=(a_1, a_2, a_3)$ and $\mathbf{b}=\mathbf{e}\times\mathbf{a}=(b_1, b_2, b_3)$, then g_s is a function of n_1 and n_2, and $\frac{\partial n_3}{\partial n_1}=-\frac{n_1}{n_3}\ \frac{\partial n_3}{\partial n_2}=-\frac{n_2}{n_3}$.

$$\frac{\partial g_s}{\partial n_1}=-W_1(\mathbf{n}\cdot\mathbf{e})(e_1-e_3\frac{n_1}{n_3})-W_2(\mathbf{n}\cdot\mathbf{a})(a_1-a_3\frac{n_1}{n_3}) \tag{A1}$$

$$\frac{\partial g_s}{\partial n_1}=-W_1(\mathbf{n}\cdot\mathbf{e})(e_2-e_3\frac{n_2}{n_3})-W_2(\mathbf{n}\cdot\mathbf{a})(a_2-a_3\frac{n_2}{n_3}) \tag{A2}$$

$$\begin{aligned}\frac{\partial^2 g_s}{\partial n_1^2}=&-W_1\left(e_1-e_3\frac{n_1}{n_3}\right)^2+W_1(\mathbf{n}\cdot\mathbf{e})e_3\frac{n_3^2+n_1^2}{n_3^3}\\&-W_2\left(a_1-a_3\frac{n_1}{n_3}\right)^2+W_2(\mathbf{n}\cdot\mathbf{a})a_3\frac{n_3^2+n_1^2}{n_3^3}\end{aligned} \tag{A3}$$

$$\begin{aligned}\frac{\partial^2 g_s}{\partial n_2^2}=&-W_1\left(e_2-e_3\frac{n_2}{n_3}\right)^2+W_1(\mathbf{n}\cdot\mathbf{e})e_3\frac{n_3^2+n_2^2}{n_3^3}\\&-W_2\left(a_2-a_3\frac{n_2}{n_3}\right)^2+W_2(\mathbf{n}\cdot\mathbf{a})a_3\frac{n_3^2+n_2^2}{n_3^3}\end{aligned} \tag{A4}$$

$$\begin{aligned}\frac{\partial^2 g_s}{\partial n_1 n_2}=&-W_1\left(e_2-e_3\frac{n_2}{n_3}\right)\left(e_1-e_3\frac{n_1}{n_3}\right)+W_1(\mathbf{n}\cdot\mathbf{e})e_3\frac{n_1n_2}{n_3^3}\\&-W_2\left(a_2-a_3\frac{n_2}{n_3}\right)\left(a_1-a_3\frac{n_1}{n_3}\right)+W_2(\mathbf{n}\cdot\mathbf{a})a_3\frac{n_1n_2}{n_3^3}.\end{aligned} \tag{A5}$$

The solutions of $\frac{\partial g_s}{\partial n_1}=0$ and $\frac{\partial g_s}{\partial n_2}=0$ are as follows.

(i) For $\mathbf{n}=\mathbf{e}$:
Here, $e_1-e_3\frac{n_1}{n_3}=e_1-e_3\frac{e_1}{e_3}=0$, while $\mathbf{a}=\mathbf{e}\times\mathbf{v}=\mathbf{n}\times\mathbf{v}$, so $\mathbf{a}\perp\mathbf{n}$, $\mathbf{n}\cdot\mathbf{a}=0$.

(ii) For $\mathbf{n}=\mathbf{a}$:
Here, $a_1-a_3\frac{n_1}{n_3}=a_1-a_3\frac{a_1}{a_3}=0$, while $\mathbf{n}=\mathbf{a}=\mathbf{e}\times\mathbf{v}$, so $\mathbf{n}\perp\mathbf{e}$, $\mathbf{n}\cdot\mathbf{e}=0$.

(iii) For $\mathbf{n}=\mathbf{e}\times\mathbf{a}=\mathbf{e}\times(\mathbf{e}\times\mathbf{v})=\mathbf{b}$:
Here, $\mathbf{n}\perp\mathbf{e}$, $\mathbf{n}\perp\mathbf{a}$, so $\mathbf{n}\cdot\mathbf{e}=0$ and $\mathbf{n}\cdot\mathbf{a}=0$.

Using the expressions (A1–A5), one can draw the following conclusions [29]. (i) For $W_1>0$ and $W_2>0$, the anchoring energy g_s has minimum value for the solutions $\mathbf{n}=\mathbf{e}$ and $\mathbf{n}=\mathbf{a}$. (ii) For $W_1<0$ and $W_2<0$, the anchoring energy g_s is minimum for the solution $\mathbf{n}=\mathbf{b}$.

References

[1] Blinov, L. M., and Chigrinov, V. G., 1994, *Electro-optic Effects in Liquid Crystal Materials* (New York: SpringerVerlag).
[2] Papini, A., and Papoular, M., 1969, *J. Phys. (Paris) Colloq.* 30, C4–54.
[3] Sonin, A. A., 1995, *The Surface Physics of Liquid Crystals* (Gordon and Breach).
[4] Palermo, V., Biscarini, F., and Zannoni, C., 1998, *Phys. Rev. E*, **57,** 2519.
[5] Steizer, J., Longa, L., and Trebin, H. R., 1997, *Phys. Rev. E*, **55,** 7085.
[6] Seidin, R., Horneich, R. M., and Aliender, D. W., 1997, *Phys. Rev. E*, **55,** 4302.
[7] Schuddeboom, P. C., and Jerome, B., 1997, *Phys. Rev. E*, **56,** 4294.
[8] Ondris-Crawford, R. J., Crawford, G. P., Zumer, S., and Doane, J. W., 1993, *Phys. Rev. Lett.*, **70,** 194.
[9] Leslie, F. M., 1970, *Mol. Cryst. liq. Cryst.*, **12,** 57.
[10] Schadt, M., and Helfrich, W., 1971, *Appl. Phys. Lett.*, **18,** 127.
[11] Nehring, J., Kmetz, A. R., and Scheffer, T. J., 1976, *J. Appl. Phys.*, **47,** 850.
[12] Yang, K. H., 1983, *J. Appl. Phys. Lett.*, **54,** 6864.
[13] Yang, K. H., 1983, *Jpn. appl. Phys, Lett.*, **22,** 389.
[14] Yang, K. H., 1983, *Appl. Phys. Lett.*, **43,** 171.
[15] Becker, M. E., Nehring, J., and Scheffer, T. J., 1985, *J. appl. Phys.*, **57,** 4539.
[16] Hirning, R., Funk, W., Trebin, H. R., Schmidt, M., and Schmiedel, H., 1991, *J. appl. Phys.*, **70,** 4211.
[17] Sugimura, A., and Ou-Yang, Z., 1995, *Phys. Rev. E*, **51,** 784; Sugimura A., Luckhurst G. R., and Ou-Yang Z., 1995, *Phys. Rev. E*, **52,** 681.
[18] Sonin, A. A., 1995, *The Surface Physics of Liquid Crystals* (London: Gordon and Breach).
[19] Becia, T., Frunza, S., Moldovan, R., and Stoenescu, D. N., 1997, *Mol. Cryst. liq. Cryst. Sci. Technol., A*, **301,** 39.
[20] Zhao, W., Wu, C.-X., and Iwamoto, M., 2000, *Phys. Rev. E*, **62,** R1481.
[21] Zhao, W., Wu, C.-X., and Iwamoto, M., 2001, *Mol. Cryst. liq. Cryst.*, **367,** 231.
[22] Zhao, W., Wu, C.-X., and Iwamoto, M., 2002, *Phys. Rev. E.*, **65,** 031709.
[23] Bryan-Brown, G. P., Brown, C. V., Sage, I. C., and Hui, V. C., 1998, *Nature*, **392,** 365.
[24] Stöhr, J., Samant, M. G., Cossy-Favre, A., Díaz, J., Momoi, Y., Odahara, S., and Nagata, T., 1998, *Macromolecules*, **31,** 1942.
[25] Weiss, K., Wöll, C., Böhm, E., Fibranz, B., Fortmann, G., Peng, B., Scheumann, V., and Johannsmann, D., 1998, *Macromolecules*, **31,** 1930.
[26] Weiss, K., Wöll, C., and Johannsmann, D., 2000, *J. Chem. Phys.*, **113,** 11297.
[27] De Gennes, P. G., 1974, *The Physics of Liquid Crystals*, (Oxford University Press), p. 345.
[28] Elggots, L., 1980, *Differential Eqations and Variation Calculus* (MIR: Moscow).
[29] Smirnow, V., 1975, *Cours de Mathematigue Superieures,* Vol. IV (MIR: Moscow).