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# Alternative method of investigating surface torsional anchoring energy for pure nematic liquid crystals

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The investigation of the surface anchoring energy for nematic liquid crystals has always been an important branch of liquid crystal physics. By measuring the twist angle in the twist cell and the surface torsional angle between the rubbing direction and the liquid crystal director at the substrate boundary, an alternative measuring method of the surface torsional anchoring energy for pure nematic liquid crystals without chiral materials is given. The torsional anchoring energy of the interface between 4-*n*-pentyl-4′-cyanobiphenyl and rubbed polyimide is determined.

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## I. INTRODUCTION

The surface alignment of nematic liquid crystal molecules on a treated substrate is an important and inevitable process for preparing experimental samples and practical devices. The investigation for the mechanism of the liquid crystal molecules orientation has always fascinated a lot of scientists, and the surface anchoring energy is a key parameter in their studies.

Many methods of measuring the surface anchoring energy have been given, such as surface disclination [1,2], Fréedericksz transition [3,4], high field [5,6], etc. Indeed, they play an important role in the investigation for surface anchoring of liquid crystals. However, the methods noted above are mostly used to measure the polar anchoring energy; information concerning the torsional anchoring energy is relatively scarce. Sato, Sato, and Uchida investigated the relationship between the rubbing strength and the surface torsional anchoring of nematic liquid crystals by Cano wedge cell [7], but chiral materials had been doped in their experimental liquid crystal materials. Oh-ide, Kuniyasu, and Kobayashi measured the torsional surface coupling strength using high magnetic field [8]. In this paper we measure the surface torsional anchoring energy of pure nematic liquid crystals without chiral materials for the case without an extra field.

## II. THEORY

As we know, according to Frank's elastic theory a liquid crystal is an elastic fluid and the state of the even and consistent alignment of the liquid crystal molecules is the state of the minimum of the bulk energy, which is the most stable state of liquid crystals. When the rubbing directions on both substrates in the cell have a cross angle to each other, the nematic liquid crystals injected in the cell also form a twist structure by the surface anchoring force. If the surface anchoring strength is weak, the direction of the surface orientation of liquid crystals deviates from the rubbing direction due to a spontaneous twisting elastic power of nematic liquid crystals. This deviated angle is determined by the balance between the twisting elastic power and the torsional anchoring energy; from this angle, the torsional anchoring energy can be calculated using the elastic theory.

In the twist liquid crystal cell, the free energy per unit area is obtained by the sum of the bulk elastic energy $f_b$ and the surface energy $f_s$ as in the following formula:

$$f=f_b+2f_s \ , \tag{1}$$

where

$$f_b=\tfrac{1}{2}K_{22}(\psi_a/d)^2 d \ , \tag{2}$$

$$f_s=\tfrac{1}{2}E_T \sin^2\varphi_s \ . \tag{3}$$

Here, $K_{22}$ is the twist elastic constant, $d$ is the cell gap, $E_T$ is the torsional anchoring energy, $\varphi_s$ is the deviation of the director at the surface from the rubbing direction, and $\psi_a$ is the actual twist angle of the director in the cell. The relation between $\psi_a$ and $\varphi_s$ can be expressed by the following equation:

$$2\varphi_s=\psi_r-\psi_a \ , \tag{4}$$

where $\psi_r$ is the angle between the two rubbing directions on both substrates.

The director orientation in the cell is obtained by minimizing $f$, or $\delta f/\delta\varphi_s=0$, which gives the torque balance equation as

$$K_{22}(\psi_a/d)=\tfrac{1}{2}E_T \sin 2\varphi_s \ . \tag{5}$$

From this equation, the surface torsional energy is expressed as

$$E_T=(2K_{22}\psi_a)/(d \sin 2\varphi_s) \ . \tag{6}$$

Equation (6) can be rewritten by substituting Eq. (4) as

$$E_T=(2K_{22}\psi_a)/[d \sin(\psi_r-\psi_a)] \ . \tag{7}$$

Equation (7) indicates that $E_T$ can be measured if the cell gap, the actual twist angle, and the angle between the rubbing directions in the cell are known. Figures 1 and 2 clearly illustrate the theoretical relations among $E_T$, $\psi_r$, and $\varphi_s$.

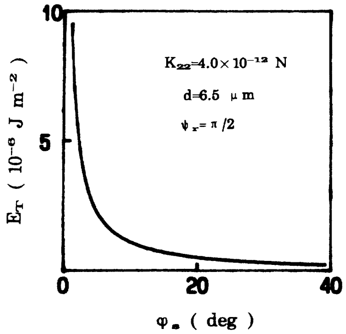

FIG. 1. The theoretical relation between $E_T$ and $\varphi_s$.

The actual twist angle and the cell gap may be measured by the experiments described by Lien [9] and Lien and Takano [10], where they used the Jones optical propagation matrix.

According to the Jones optical propagation matrix, the optical transmission of twist nematic liquid crystal cell between two polarizers can be described by the following formula:

$$T=\left\{\frac{1}{\sqrt{1+u^2}}\sin(\sqrt{1+u^2}\psi_a)\sin(\psi_a-\psi_p)+\cos(\sqrt{1+u^2}\psi_a)\cos(\psi_a-\psi_p)\right\}^2+\frac{u^2}{\sqrt{1+u^2}}\sin^2(\sqrt{1+u^2}\psi_a)\cos^2(\psi_a+2\psi_0-\psi_p), \quad (8)$$

where

$$u=\frac{\pi d}{\lambda\psi_a}\left[\frac{n_e}{\sqrt{1+w\sin^2\theta}}-n_o\right],$$

and

$$w=\left[\frac{n_e}{n_o}\right]^2-1,\quad \theta=\frac{1}{d}\int_0^d\theta(z)dz .$$

Here, $\psi_a$ is the twist angle, $\psi_0$ is the angle of entrance of the liquid crystal director with respect to the transmission axis of the entrance polarizer, $\psi_p$ is the angle between the transmission axes of the exit and entrance polarizer, $n_o$ and $n_e$ are the ordinary and extraordinary indices of refraction of liquid crystals, respectively, and λ is the wavelength of incident light. If $\theta_s \le 2°$, then $\theta=\theta_s$, in which $\theta_s$ is the pretilt angle of liquid crystals.

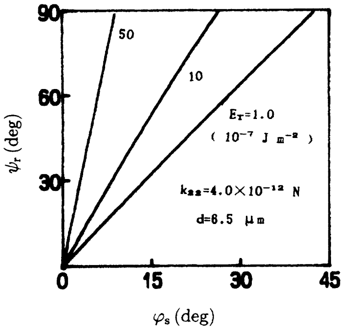

FIG. 2. The theoretical relation between $\psi_r$ and $\varphi_s$.

The transmission $T$ can be minimized with respect to $\psi_p$ and $\psi_0$ by

$$\frac{\delta T}{\delta\psi_0}=0,\quad \frac{\delta^2 T}{\delta\psi_0^2}>0,\quad \frac{\delta T}{\delta\psi_p}=0,\quad \frac{\delta^2 T}{\delta\psi_p^2}>0 . \quad (9)$$

From Eq. (8), we can get the minimal transmission conditions

$$\psi_a+2\psi_0-\psi_p=(m/2)\pi , \quad (10)$$

where $m$ is the odd integer, and

$$(1+u^2)\cos^2(\sqrt{1+u^2}\psi_a)\sin(2\psi_a-2\psi_p)-\sin^2(\sqrt{1+u^2}\psi_a)\sin(2\psi_a-2\psi_p)-\sqrt{1+u^2}\sin(2\sqrt{1+u^2}\psi_a)\cos(2\psi_a-2\psi_p)=0 . \quad (11)$$

The optical phase difference from the twist nematic cell can be related by

$$\tan(\delta_x-\delta_y)=A/B , \quad (12)$$

where

$$A=-u\sin(2\sqrt{1+u^2}\psi_a) ,$$

$$B=\sqrt{1+u^2}\cos(2\psi_a)\cos(2\sqrt{1+u^2}\psi_a)+\sin(2\psi_a)\sin(2\sqrt{1+u^2}\psi_a) .$$

Here, $\delta_x$ and $\delta_y$ are the optical phases of the $X$ axis and $Y$ axis.

$\psi_p$ under the minimal transmission can be measured easily by rotating the polarizers and the liquid crystal cells. The phase difference $(\delta_x-\delta_y)$ can be determined by using a compensator. After $\psi_p$, the phase difference is known; by solving Eqs. (11) and (12), the actual twist angle $\psi_a$ and the cell gap $d$ can be determined. The measurement uncertainty of this method is within 1% for the result of the cell gap and within 1° for the result of the twist angle [9,10].

## III. TORSIONAL ANCHORING ENERGY AT 4-*n*-PENTYL-4′-CYANOBIPHENYL (5CB) -POLYIMIDE INTERFACE

The method was applied to an interface between liquid crystal 5CB and rubbed polyimide (which was supplied by Changchun Institute of Applied Chemistry, Chinese Academy of Sciences). The experimental cells were prepared as 0°–90° cells ($\psi_r=0-\pi/2$). The rubbing strength parameter $\mathfrak{R}$ was expressed by $\mathfrak{R}=Nl[2\pi rn/(60v)-1]$, where $l$, $N$, $r$, $n$, and $v$ stand for the depth of the distorted portion of the fabric on a rubbing machine, the repeated times of the rubbing, the radius of the drum, the rotation rate of the drum, and the translating velocity of the substrate, respectively. In the experiments, the rubbing strength is $\mathfrak{R}=10$ cm.

Using the crystal rotation, we measured that the pretilt

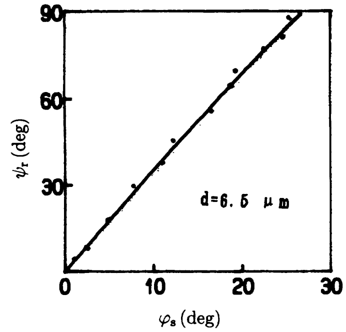

FIG. 3. The experimental results of $\psi_r$ and $\varphi_s$.

angle of liquid crystals is 1°.

Figure 3 shows the experimentally determined results of $\psi_x$ and $\varphi_s$. From this relation, we obtain the surface torsional anchoring energy $E_T$ as

$$E_T=(1.0\pm0.1)\times10^{-6}\ \mathrm{J\,m^{-2}}\ .$$

This result is the same as other reports [8,11].

## IV. DISCUSSION

In order to examine the effect of the uncertainties in $\psi_a$ and $d$ on the resultant torsional anchoring energy $E_T$, from Eq. (7), we can easily get the error in $E_T$ as

$$\delta E_T=E_T\{[(1/\psi_a)+\cot(\psi_r-\psi_a)]\delta\psi_a-(1/d)\delta d\}\ , \tag{13}$$

$$\delta E_T/E_T=[(1/\psi_a)+\cot(\psi_r-\psi_a)]\delta\psi_a-(1/d)\delta d\ . \tag{14}$$

In accordance with the method to measure the twist angle and cell gap, the relative errors in $\psi_a$ and $d$ are $\delta\psi_a=0.017$ rad and $\delta d/d=0.01$, respectively. Then, we can determine that the errors in $E_T$ are 3–10% if the twist angle is 90°–35°, and that the errors are more than 10% if the twist angle is less than 35°. It is clearly shown that, for this measuring method, the obtained result of $E_T$ is more accurate when the twist angle is more than 35°. Additionally, this method, without extra field, was avoided bringing in ions or the flexoelectric effect under high field.

On the other hand, at planar cells, considering the inversion symmetry of nematic liquid crystals, we may expand the surface energy function in a power series of $\sin^2\varphi_s$:

$$f_s=\tfrac{1}{2}\sin^2\varphi_s\left[E_T+\sum_{n=1}^{\infty}E_n\sin^{2n}\varphi_s/(n+1)\right]\ , \tag{15}$$

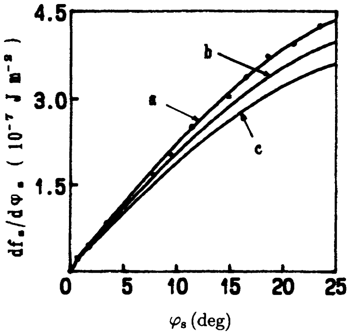

FIG. 4. Second-order fitting of the surface energy function by the function of the form $f_s=\frac{1}{2}E_T\sin^2\varphi_s+\frac{1}{4}E_1\sin^4\varphi_s$. (a) $E_T=1.3\times10^{-6}$ J m$^{-2}$ and $E_1=-8.9\times10^{-7}$ J m$^{-2}$; (b) $E_T=1.2\times10^{-6}$ J m$^{-2}$ and $E_1=-8.9\times10^{-7}$ J m$^{-2}$; and (c) $E_T=1.1\times10^{-6}$ J m$^{-2}$ and $E_1=-8.9\times10^{-6}$ J m$^{-2}$.

where $E_T$ and $E_n$ are the coefficients of expansion, which can be expected to more or less reflect the symmetry of the interaction working at the interface. Therefore,

$$df_s/d\varphi_s=\tfrac{1}{2}\sin2\varphi_s\left[E_T+\sum_{n=1}^{\infty}E_n\sin^{2n}\varphi_s\right]\ . \tag{16}$$

As long as the van der Waals [12,13] or steric [14] interaction is dominant, the higher-order terms in the expansion are considered to be relatively unimportant. Figure 4 shows two trial functions incorporating the second higher-order term.

From the torque balance condition $\delta f/\delta\varphi_s=0$, we can obtain

$$df_s/d\varphi_s=\tfrac{1}{2}K_{22}(\psi_r-2\varphi_s)/d\ . \tag{17}$$

Using the relations indicated by Fig. 3 and Eq. (17), the experimental results of $df_s/d\varphi_s$ are obtained and shown in Fig. 4.

According to Fig. 4, the fitted second-order coefficient $E_1$ with the experimental results is a negative: $E_1=-8.9\times10^{-7}$ J m$^{-2}$ and $E_T=1.3\times10^{-6}$ J m$^{-2}$.

## V. CONCLUSIONS

This paper has given an alternative measuring method of the surface torsional anchoring energy for pure nematic liquid crystals (without chiral materials) by measuring the actual twist angle in the twist cell and the surface torsional angle between the rubbing direction and the liquid crystal director at the substrate boundary. The torsional surface energy at the 5CB-polyimide interface was found to be well fitted by the function of the form $\frac{1}{2}E_T\sin^2\varphi_s+\frac{1}{4}E_1\sin^4\varphi_s$ with $E_T\sim1.3\times10^{-6}$ J m$^{-2}$ and $E_1\sim-8.9\times10^{-7}$ J m$^{-2}$.

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