



Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and
subscription information:

<http://www.tandfonline.com/loi/gmcl19>

Temperature Dependence of Pretilt Angle in Nematic Liquid Crystal Cell

Takashi Sugiyama^{a b}, Seiyu Kuniyasu^{a b} & Shunsuke Kobayashi^a

^a Department of Electronic Engineering, Faculty of Technology,
Tokyo University of Agriculture and Technology, 2-24-16
Nakamachi, Koganei-ski, Tokyo, 184, Japan

^b Stanley Electric Co Ltd., Yokohama, Kanagawa, 225, Japan

Version of record first published: 24 Sep 2006.

To cite this article: Takashi Sugiyama, Seiyu Kuniyasu & Shunsuke Kobayashi (1993): Temperature Dependence of Pretilt Angle in Nematic Liquid Crystal Cell, Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals, 231:1, 199-214

To link to this article: <http://dx.doi.org/10.1080/10587259308032506>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.tandfonline.com/page/terms-and-conditions>

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

Temperature Dependence of Pretilt Angle in Nematic Liquid Crystal Cell

TAKASHI SUGIYAMA,[†] SEIYU KUNIYASU[†] and SHUNSUKE KOBAYASHI

Department of Electronic Engineering, Faculty of Technology, Tokyo University of Agriculture and Technology, 2-24-16 Nakamachi, Koganei-ski, Tokyo 184, Japan

(Received September 22, 1992; in final form November 16, 1992)

The pretilt angle generated in a nematic liquid crystal medium filled in a sandwich cell is shown to decrease with increasing temperature regardless of the ways for generating the pretilt angle. Numerical analyses of spatial and temperature dependence of pretilt angles on a model surface have been done based on a phenomenological continuum theory; the analyses are shown to explain successfully the observed temperature dependence of the pretilt angles.

Keywords: pretilt angle, temperature dependence, nematic liquid crystal, branched polyimide, branchless polyimide

1. INTRODUCTION

The investigation on the alignment of the liquid crystals (LCs) on treated substrates are of importance both for scientific and practical points of view.^{1,2} Among them the research on the way to generate the pretilt angle and on its mechanism is a current theme in the LC study, since the existence of the tilt bias called the pretilt angle is necessary to avoid the appearance of the reverse tilt disclinations in the ordinary LC devices, such as tunable birefringent and ordinary twisted nematic types,³ and further to eliminate the appearance of the stripe domains in a super-twisted nematic liquid crystal (STN) device.^{4,5,6}

A low pretilt angle, say 1 ~ 2 degrees, that is necessary for fabricating ordinary TN-LCD can be generated by performing rubbing on ordinary polymer films such as polyimide (PI)^{7,8}; on the other hand, high pretilt angles of 5 degrees or more that is necessary, for example, in the fabrication of defect-free STN-LCD can be generated by using properly rubbed alkylamine branched PI.^{9,10,11} Alternative ways to generate a medium or high pretilt angles are to use rubbed alkylamine-blended PI,¹² chromic-salt-doped PI,¹³ and PI containing trifluorocarbon moieties.¹⁴

It is well known that the pretilt angle in an NLC medium filled in a sandwich

[†]On leave from Stanley Electric Co Ltd., Yokohama, Kanagawa 225, Japan.

type cell that is generated by the oblique evaporation technique of SiO decreases with increasing temperature.^{15,16}

Unlike ordinary direct view type LCDs, the LCD panels which are being utilized as a component of a projection set are heated up to 50 to 60°C. Therefore, there occurs sometimes reverse tilt disclinations in these device cells due to the decrease of the pretilt angle with temperature.

The problem of the temperature variation of the pretilt angle has been discussed by several investigators already,^{17,18,19} however due to the advent of the above mentioned phenomena we need to reinvestigate this problem again.

This research work has been done with the aim of providing a model of the generation of the pretilt angle and a theoretical calculation for explaining the temperature dependence of the pretilt angle in an NLC cell with rubbed alkyl-branchless and alkyl-branched polyimide orientation films. The discussion is also made on the case where obliquely evaporated SiO films are used.

2. MODELS OF PRETILTED CONFORMATIONS OF NEMATIC LIQUID CRYSTALS

2.1 Conformation with Low Tilt Angle Prepared by Using the Rubbed Branchless Polyimide

A low pretilt angle in an NLC prepared by rubbing technique is thought to be induced by a surface structure generated through the stick slip process which occurs often in the tribology.^{11,20} ‡

The schematic drawings for the surface structure of the worked surface and the molecular conformation in the NLC medium that is suggested in this paper are shown in Figures 1(a) and 1(b). The worked surface is assumed to consist of repeated slopes. Each NLC molecule is represented by a rod. Those rod-like molecules located just in the vicinity of the orientation film are assumed to be anchored in terms of the surface interaction between LC molecules and the substrate. In the bottom region the arrangement of the rod-like molecules is formed in such a way that reflects the spatial variation of the surface structure; while in the region of the deep off surface the molecules are assumed to take a uniform direction so that the medium is free from elastic deformation, then the director in this region determines the pretilt angle θ_p .

2.2 Conformation with High Tilt Angle Prepared by Using the Rubbed Alkyl-Branched Polyimide

In the case where the alkyl-branched polyimide films are used, the pretilt angle is thought to be generated in terms of the steric interaction between the rod-like LC molecules and the branches.¹¹ (A schematic drawing for this LC molecular con-

‡As an alternative to this model, Geary *et al.* suggested that there is an inclined easy axis that is mechanically induced due to the rubbing,²¹ the research based on the inclined easy axis is now under way, and it will be published elsewhere.

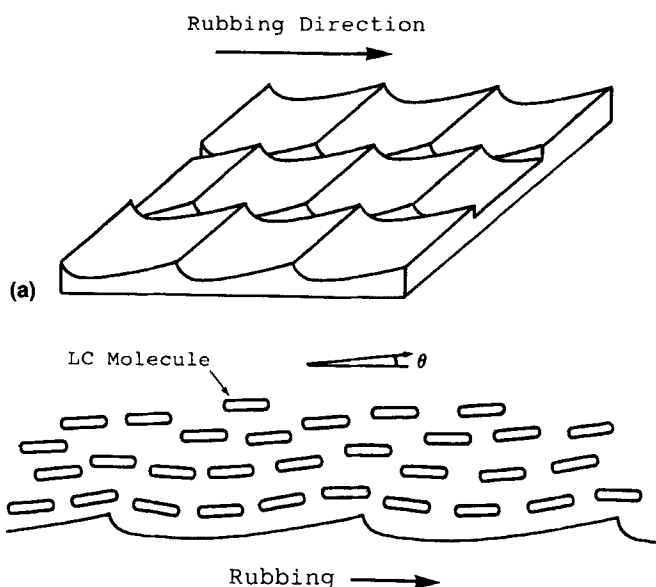


FIGURE 1 An illustrative drawing for the worked surface structure of the branchless polyimide due to unidirectional rubbing (a) and the molecular conformation of the nematic liquid crystals (b).

formation is presented in Reference 11.) The LC molecules in the neighborhood of the alkyl branches are assumed to take almost the same direction as those of the branches to minimize the excluded volume.²² Therefore, in the same manner as for the branchless substrate, the LC molecules in the bottom region reflect the spatial variation of the surface topography; further, in the region of the off surface the LC molecules are assumed to take a uniform direction, and it gives rise to form a pretilted conformation with an angle θ_p . In this case the general direction of the director of the nematic medium projected on the substrate may be determined by the direction of the main chain of the rubbed polymer, except for a special case such as polystyrene, while the branches may play a major role in determining the pretilt angles.

3. EXPERIMENTAL METHOD AND RESULTS

The sample cells used in the experiment consisted of two parallel glass plates whose inside surfaces were coated with polyimide films with or without alkyl branches, which were rubbed in an antiparallel way; the space was filled with an NLC, 5CB, having 70 μm thickness. The pretilt angles of the sample cells were controlled by changing the rubbing strength[§] which was monitored in terms of the induced birefringence occurring in the orientation films.¹⁰ The sample cells used in this measurement were prepared by strong rubbing on the branchless polyimide, and strong and weak rubbing on the branched polyimide, which give rise to yield the pretilt

[§]The definition of the rubbing is given in Reference 8.

angles of 1.7, 3.1, and 7.7 degree at a low temperature, 25°C, respectively. The samples prepared in this way are designated as A, B and C, respectively.

The sample cell was set in a temperature-controlled housing in a system for measuring pretilt angles using the crystal rotation method.²³ This method was supplemented by an alternative method in which the variation of the optical retardation with the rotation angle was measured; the maximum value of the retardation is attributable to the pretilt angle. The agreement between these two methods was excellent. The accuracy of the temperature control was $\pm 0.1^\circ\text{C}$.

The temperature variations of the measured pretilt angles obtained in this way for samples A, B and C are shown in Figure 2, expressed by filled circles, open circles and open triangles, respectively. All the pretilt angles of these three sample cells are shown to decrease monotonically with increasing temperature in the range below the N-I point. The solid lines are drawn by theoretical calculations which will be discussed in a later section.

4. A SIMULATION FOR THE TEMPERATURE DEPENDENCE OF THE PRETILT ANGLE

The first step of our analysis is to calculate the conformation of LC molecules located in the vicinity of the surface. Then, the analytical consideration of the

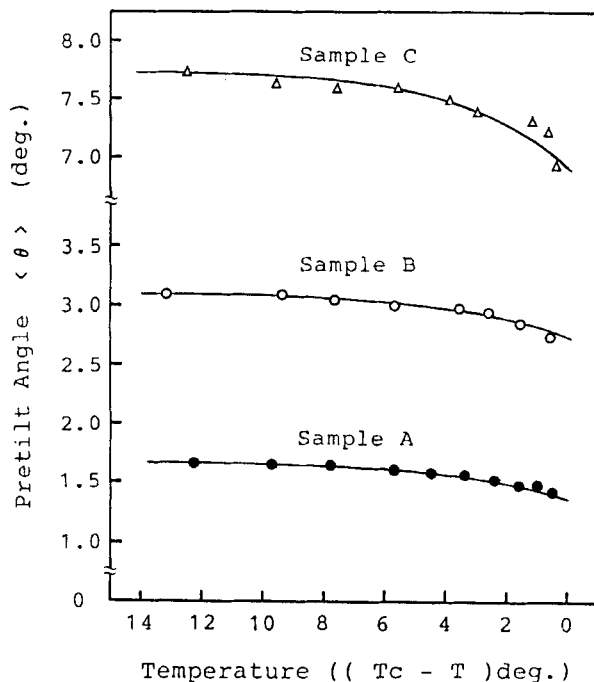


FIGURE 2 The temperature dependence of the pretilt angle below T_c . Dots represent experimental results: \bullet , sample A by strong rubbing of the branchless polyimide; \circ , sample B by strong rubbing and Δ , sample C by weak rubbing of the branched polyimide films. Solid lines are the result of the theoretically best fit.

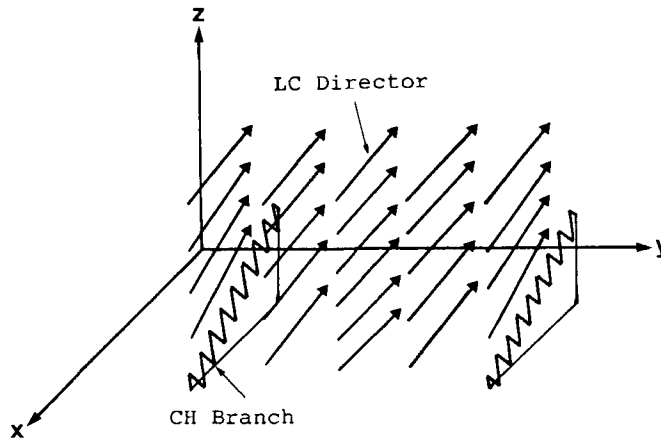


FIGURE 3 An illustrative drawing for the molecular conformation on the surface in the case of using the branched polyimide together with the coordinate system used in the theoretical calculation.

balance between two forces exerting on these molecules is done, where one is the force caused from the elastic deformation of an LC due to influence of the surface topography, and the other is the force caused from the surface anchoring energy. We assume that the surface anchoring force tend the molecules to be parallel to the local surface.

The second step is to calculate the spatial variation of the molecular conformation toward the region of the off surface. The final molecular conformation can be calculated by minimizing the total elastic free energy.

In the following, the simulation is given in the order of branched and branchless polyimide films.

4.1 An Analytical Calculation for the Molecular Conformation in the Case of Using the Branched Polyimide

Figure 3 is an illustrative drawing for a pretilted molecular conformation generated in terms of the interaction with the branches attached to the main chains of the polymer. For simplicity, we assumed that the branches distribute regularly and homogeneously. Therefore, the branches are aligned along the straight line parallel to the x axis and having a width of “ l ”, and there is no variation of LC molecules along the x axis. The LC director orients toward the x axis.

Two forces exert on the LC molecules located in the vicinity of the surface; one is that originated from the twisted deformation between two adjacent branches and the other is caused by the surface anchoring. These two forces balance in the following way||:

$$K_{22} \frac{\partial^2 \theta_1}{\partial y^2} = K \frac{\partial^2 \theta_1}{\partial z^2}, \quad (1)$$

||This model is analogous to a problem concerning the determination of the shape of a thread suspended between two poles and attracted uniformly by gravity.

where K in the right hand side is the elastic constant, we assumed one constant, (i.e. $K = K_{11} = K_{33}$, for splay and bend deformation), K_{22} is that for twist deformation, and θ_1 is the tilt angle of the LC molecules located in the vicinity of the surface.

The torque balance equation on the surface can be written as follows by taking account of the surface energy:

$$K \frac{\partial \theta_1}{\partial z} = A_\theta \sin \theta_1 \cos \theta_1, \quad (2)$$

where A_θ stands for the polar anchoring constant. Then by using this equation, Equation (1) can be read as:

$$\frac{\partial^2 \theta_1}{\partial y^2} = \frac{A_\theta^2}{K_{22}K} \sin \theta_1 \cos \theta_1 (\cos^2 \theta_1 - \sin^2 \theta_1). \quad (3)$$

The tilt angle of the LC molecule just above the branch is assumed to be equal to that of the branch (θ_b), and the molecular conformation in the vicinity of the surface can be obtained by solving Equation (3) by using the Runge-Kutta method.

Next, the state of the molecular conformation toward the region of the off surface is calculated by minimizing the free energy. Because of the symmetry of the system, the free energy (W) can be expressed

$$W = \int_0^{d/2} \int_0^{l/2} \left[\frac{1}{2} K_{22} \left(\frac{\partial \theta}{\partial y} \right)^2 + \frac{1}{2} K \left(\frac{\partial \theta}{\partial z} \right)^2 \right] dy dz, \quad (4)$$

where, “ l ” is the distance between two adjacent branches. In order to simplify the calculation, we assume the following:

$$\theta = \theta_p + (\theta_1 - \theta_p)e^{-\alpha z} \quad (5)$$

and

$$\frac{\partial \theta}{\partial y} = \left(\frac{\partial \theta_1}{\partial y} \right) e^{-\alpha z}, \quad (6)$$

where α is an adequate constant. Rearranging Equation (4) by substituting Equations (5) and (6), we have

$$W = \frac{1}{4} (1 - e^{-\alpha d}) \int_0^{l/2} \left[\frac{k_{22}}{\alpha} \left(\frac{\partial \theta_1}{\partial y} \right)^2 + K \alpha (\theta_1 - \theta_p)^2 \right] dy. \quad (7)$$

The combination of θ_p and α , which minimize the value of W in Equation (7), is obtained by a computer simulation. Providing that the value of $1/\alpha$ is sufficiently

small compared to the cell thickness, the majority of molecules in the cell are aligned in a direction characterized by θ_p . Then this angle may be taken as the pretilt angle. Furthermore, the value of α is considered to correspond to $4\pi/\lambda$ where λ is the spatial wave length of the sinusoidal surface undulation ($z = A \sin(2\pi/\lambda)y$, where A is the amplitude of the undulation), which was introduced by Berreman.²⁴

The pretilt angle caused by the surface topography can be obtained in this manner. Moreover, it is necessary to consider the temperature dependence of K and A_0 in order to calculate that of the pretilt angle. Concerning K , it is well known that K is proportional to the square of the order parameter S^2 ,²⁵ where S is an order parameter. Regarding the A_0 , various models have been proposed, among them a model based on the excluded volume effect²² which claims that the A_0 is proportional to kTS , where k and T stand for Boltzmann constant and absolute temperature, respectively. Another model based on van der Waals interaction²⁶ also claims proportionality to the S . However, the effect of the variation of T contribute only a few percent in kTS for the sample 5CB, it can be thought that A_0 is proportional to S in both cases substantially.

The reduced temperature variation of S , normalizing the value at 24°C, is obtained by measuring the optical retardation of the sample cell using the same system reported in the previous paper.¹⁰ The results for the normalized temperature dependence of the order parameters of the samples A, B, and C determined in this way are shown in Figure 4. The temperature dependence of the pretilt angle for samples B and C are shown in Figure 2 by the middle and top solid lines. These theoretical values were obtained by substituting each value listed in Table I into Equations (3) and (7). The values for K_{22} , K and A_0 in Table I are taken from those given in the literature²⁷ and previous paper.¹¹ The value of " l " is estimated

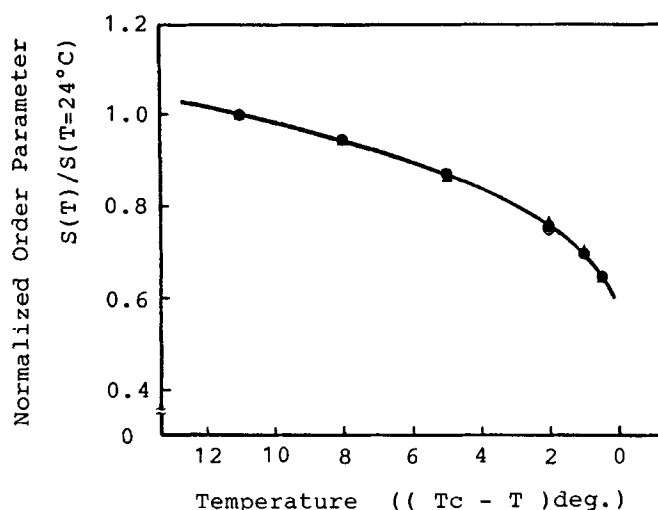


FIGURE 4 Experimental results for the temperature dependence of the normalized order parameters for the three samples: ●, strong rubbing (sample A) of the branchless polyimide; ○, strong (sample B) and △, weak rubbing (sample C) of the branched polyimide.

TABLE I

The values used in the simulation for samples B and C

| | Sample B | Sample C |
|---|-----------------------|-----------------------|
| A_9 ($T = 24^\circ\text{C}$)(J/m ²) | 1.0×10^{-3} | 1.0×10^{-3} |
| K_{22} ($T = 24^\circ\text{C}$)(N) | 4.0×10^{-12} | 4.0×10^{-12} |
| K ($T = 24^\circ\text{C}$)(N) | 8.0×10^{-12} | 8.0×10^{-12} |
| θ_b (deg) | 3.4 | 8.4 |
| l (nm) | 6.0 | 6.0 |

TABLE II

The values of α obtained by the simulation for samples B and C

| Temp. ($^\circ\text{C}$) | Sample B | Sample C |
|----------------------------|--------------------|--------------------|
| 24.0 | 8.98×10^8 | 9.04×10^8 |
| 29.0 | 9.04×10^8 | 9.05×10^8 |
| 32.0 | 9.05×10^8 | 9.08×10^8 |
| 34.0 | 9.10×10^8 | 9.10×10^8 |
| 34.5 | 9.15×10^8 | 9.15×10^8 |

by the density and length of the branch.¹¹ Moreover, θ_b is adopted to obtain the best fitting.

The values of α at the typical temperature, which were obtained in the present calculations, are listed in Table II. These values are slightly smaller than the value ($4\pi/\lambda = 2.1 \times 10^9$ [1/m]) which is suggested by Berrman's analysis, because we think that the surface undulation is not a simple sinusoidal function but contains higher harmonic components. Moreover, it is found that α increases monotonically with the temperature and shows nearly the same value regardless of the angle of the branch.

Figure 5 shows the molecular conformation in the vicinity of the surface for Sample C at $T = 24, 32$, and 34.5°C , respectively. It is found that the tilt angles of the LC molecules between two adjacent branches decrease with the increase of the temperature.

4.2 A Simulation for the Molecular Conformation in the Case of Using the Branchless Polyimide

The surface structure is assumed to be generated by stick slip, as described in subsection 2.1. The structure is characterized by the repeated slopes and the flat parts; the lengths, height, and angles of the slopes for the one unit are designated as a , b , c , h , ϕ_1 , and ϕ_2 , respectively, as shown in Figure 6. We assumed that there was no variation of the surface structure along the y axis. Then the director orientation changes along the x and z axes as illustrated in Figure 7, where the director is oriented to the x axis.

Same as for the branched film, the equation for the balance of the two forces working on the LC molecules located in the vicinity of the surface is written as:

$$K \frac{\partial^2 \theta_1}{\partial x^2} = K \frac{\partial^2 \theta_1}{\partial z^2}. \quad (8)$$

The equation for surface torque balance for the three regions can be written as follows:

$$\begin{aligned}
 K \frac{\partial \theta_1}{\partial z} &= A_0 \sin(\theta_1 - \phi_1) \cos(\theta_1 - \phi_1): \quad 0 \leq x \leq a \\
 K \frac{\partial \theta_1}{\partial z} &= A_0 \sin \theta_1 \cos \theta_1: \quad a \leq x \leq a + b \\
 K \frac{\partial \theta_1}{\partial z} &= A_0 \sin(\theta_1 - \phi_2) \cos(\theta_1 - \phi_2): \quad a + b \leq x \leq a + b + c. \quad (9)
 \end{aligned}$$

Equation (9) substituted into Equation (8) gives

$$\begin{aligned}
 \frac{\partial^2 \theta_1}{\partial x^2} &= \frac{A_0^2}{k^2} \sin(\theta_1 - \phi_1) \cos(\theta_1 - \phi_1) \\
 &\quad \cdot \{\cos^2(\theta_1 - \phi_1) - \sin^2(\theta_1 - \phi_1)\}: \quad 0 \leq x \leq a \\
 \frac{\partial^2 \theta_1}{\partial x^2} &= \frac{A_0^2}{k^2} \sin \theta_1 \cos \theta_1 \\
 &\quad \cdot (\cos^2 \theta_1 - \sin^2 \theta_1): \quad a \leq x \leq a + b \\
 \frac{\partial^2 \theta_1}{\partial x^2} &= \frac{A_0^2}{K^2} \sin(\theta_1 - \phi_2) \cos(\theta_1 - \phi_2) \\
 &\quad \cdot \{\cos^2(\theta_1 - \phi_2) - \sin^2(\theta_1 - \phi_2)\}: \quad a + b \leq x \leq a + b + c. \quad (10)
 \end{aligned}$$

The molecular conformation in the surface region along the x axis is obtained by a computer simulation using the Runge-Kutta method. Moreover the free energy is obtained to decide the state of the molecular conformation toward the region of the off surface. Then, because of the symmetry of the system, the free energy (W) can be expressed

$$W = \int_0^{d/2} \int_0^{a+b+c} \left[\frac{1}{2} K \left(\frac{\partial \theta}{\partial x} \right)^2 + \frac{1}{2} K \left(\frac{\partial \theta}{\partial z} \right)^2 \right] dx dz, \quad (11)$$

and we assumed the following in the same manner as for the branched case:

$$\theta = \theta_p + (\theta_1 - \theta_p) e^{-\alpha z} \quad (12)$$

$$\frac{\partial \theta}{\partial x} = \left(\frac{\partial \theta_1}{\partial x} \right) e^{-\alpha z} \quad (13)$$

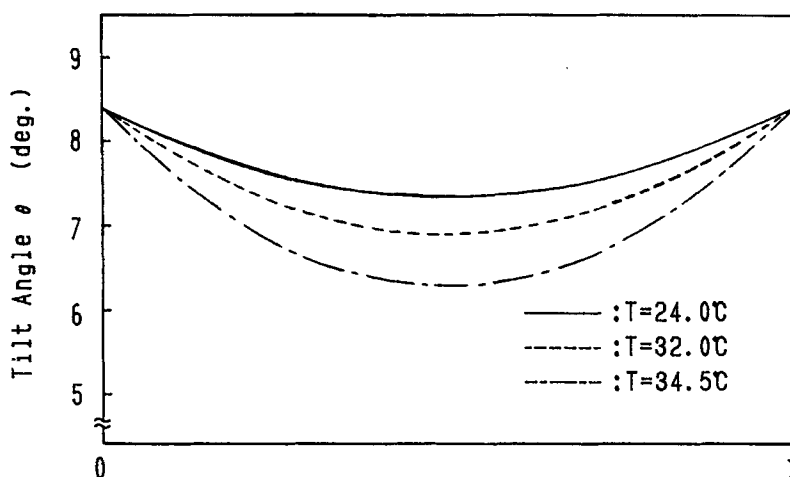


FIGURE 5 The result of the theoretical calculation of spatial variations of the tilt angles of NLC molecules located in the vicinity of the surface for various temperatures in the case of using the branched polyimide film.

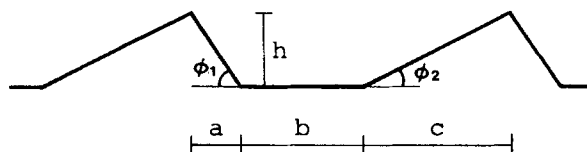


FIGURE 6 A schematic drawing for the surface structure of the branchless polyimide film generated by stick slip.

Rearranging Equation (11) by substituting Equations (12) and (13), we obtain

$$W = \frac{1}{4} (1 - e^{-\alpha d}) \int_0^{a+b+c} \left[\frac{k}{\alpha} \left(\frac{\partial \theta_1}{\partial x} \right)^2 + K\alpha (\theta_1 - \theta_p)^2 \right] dx. \quad (14)$$

The combination of θ_p and α minimizing Equation (14) is decided. If the value of $1/\alpha$ is sufficiently small compared to the cell thickness, then θ_p can be regarded as the pretilt angle.

The simulation was done by assuming that K and A_θ are proportional to $S^{2.25}$ and S , respectively. We succeeded in obtaining the best fitting for the observation for a cell with branchless polyimide films by choosing the values of parameters listed in Table III; where the values for K and A_θ are taken from those given in the literature²⁷ and previous paper,¹¹ and the periodicity of the surface structure ($a + b + c$) is taken as about 50 nm, which is 35 times larger than the length of the LC molecules (1.5 nm). The grounds for the value of the repeated structure is discussed in the appendix. Further, the parameters that determine the shape of the triangle (i.e. a , b , c , h , ϕ_1 and ϕ_2 in Figure 6) are chosen so as to fit to the pretilt angle at a low temperature. Consequently, we obtained a best-fit temperature

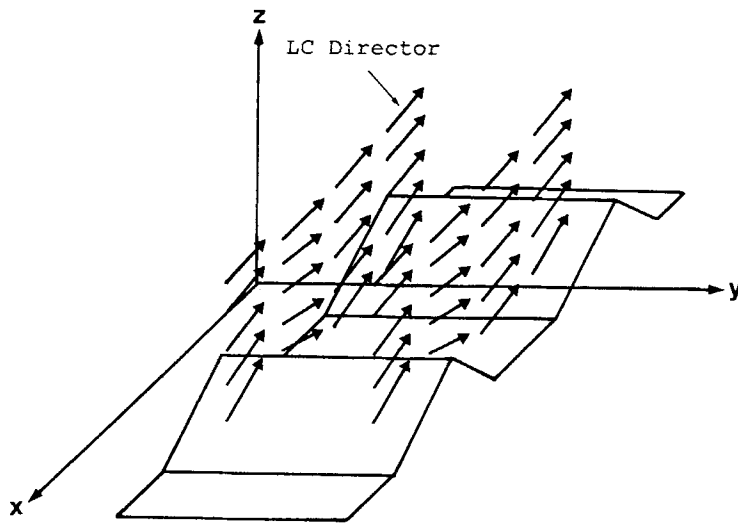


FIGURE 7 An illustrative drawing for the molecular conformation on the surface in the case of using the branchless polyimide film together with the coordinate system used in the theoretical calculation.

TABLE III

The values used in the simulation for sample A

| | |
|---|-----------------------|
| A_0 ($T = 24^\circ\text{C}$)(J/m^2) | 1.0×10^{-3} |
| K ($T = 24^\circ\text{C}$)(N) | 8.0×10^{-12} |
| a (nm) | 4.0 |
| b (nm) | 20.0 |
| c (nm) | 26.0 |
| h (nm) | 2.4 |
| ϕ_1 (deg.) | -31.0 |
| ϕ_2 (deg.) | 5.3 |

dependence of the pretilt angle for sample A as shown by the bottom line in Figure 2. Figure 8 shows the molecular conformation in the vicinity of the surface for $T = 24, 32$ and 34.5°C , respectively. It is found to reflect the spatial variation of the surface structure with the increase of the temperature.

Moreover, the values of α obtained in this simulation at the typical temperature are listed in Table IV. In this case, because of the same reason for the branched case, these values are slightly smaller than the value ($4\pi/\lambda = 2.5 \times 10^8$ [1/m]) that is suggested by Berrman's analysis.²⁴ And it is also found that it increases monotonically with the temperature.

Through this simulation, we are able to know how the pretilt angle changes according to the variation of the surface topography. The variation of θ_p as a function of the ratio c/a is shown in Figure 9 where the height h was kept constant. The values used in this simulation were $a + c = 30 \times 10^{-9}$ m, $b = 20 \times 10^{-9}$ m, and $h = 2.4 \times 10^{-9}$ m, respectively. No pretilt occurs, particularly when this triangle is symmetrical ($c/a = 1$). Further, the direction of the pretilt is shown in accordance with that of the longer slope and the value of it is shown to increase with getting out of the symmetry.

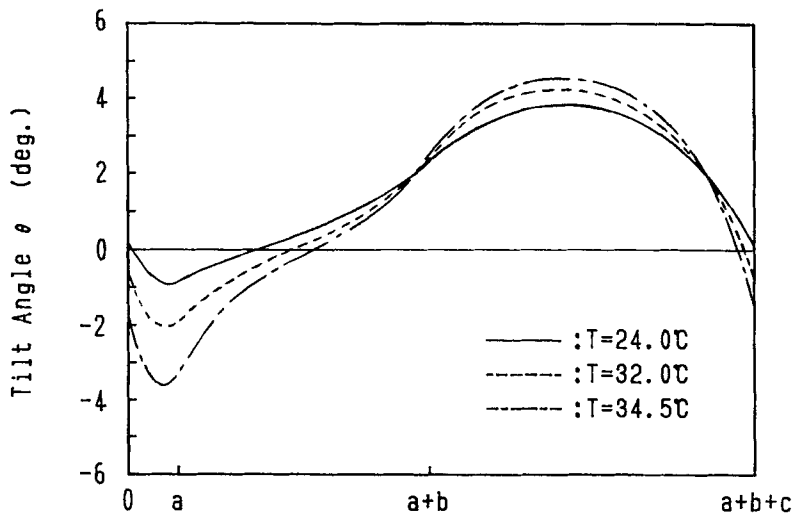


FIGURE 8 The result of the theoretical calculation of spatial variations of tilt angles of NLC molecules located in the vicinity of the surface for various temperatures in the case of using the branchless polyimide film.

TABLE IV

| The values of α obtained by the simulation for sample A | |
|--|--------------------|
| Temp. (°C) | Sample A |
| 24.0 | 1.45×10^8 |
| 29.0 | 1.49×10^8 |
| 32.0 | 1.55×10^8 |
| 34.0 | 1.64×10^8 |
| 34.5 | 1.69×10^8 |

5. COMPARISON OF THE EXPERIMENTAL DATA WITH ANALYTICAL CALCULATION AND DISCUSSION

An excellent agreement between the calculation and experimental data is seen in Figure 2; this may support the validity of the models proposed in this paper for the two types of polyimide films.

In a special case, for example, at high temperature, the tilt angle of the branch may decrease due to the melting of the branch; it may in turn accelerate the decrease of the pretilt angle of the LC medium with the temperature. However, the sample used in this experiment (5CB) has a relatively low N-I point (35°C). Therefore it may be not necessary to consider the deformation of the branches attaching to the polyimide film itself in this particular case. However, in the case where LCs with a wide nematic range were utilized, as exemplified by those for STN-LCD or projection type display, the N-I point reaches about 100°C. We therefore have to consider the temperature variation of the tilt angles of the branches due to the melting of the branches. Moreover, the slipping down of the LC molecules from

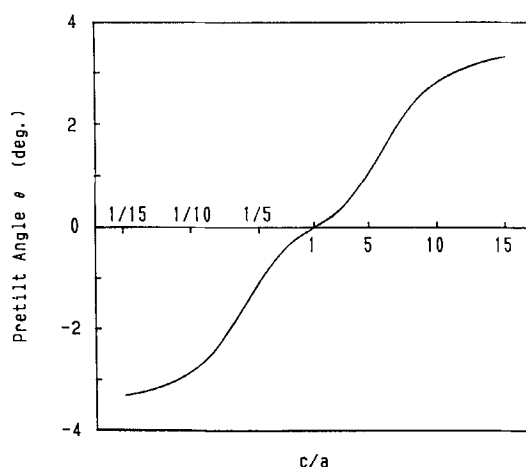


FIGURE 9 The result of the theoretical calculation for the variation of the pretilt angle as a function of a parameter characterizing the surface topography in the case of using the branchless polyimide film.

the branches due to molecular fluctuation have to be taken into account. In order to reduce the temperature variation of the pretilt angle with the increase of the temperature it is recommended to use an LC with a high clearing point and a branch with a high melting temperature.

In the present simulation, we make a clear distinction between two cases where branchless and branched polyimide are used. However, it is thought that in the former case there may exist small tilted columns and in the later case also repeated asymmetrical triangles due to the rubbing. For these reasons, there may occur almost the same behavior in the temperature variations of the pretilt angles in both cases. The model and method of calculation suggested in this work may be applied to a case where obliquely evaporated SiO films are used; however in order to explain a drastic temperature variation as observed by Van Sprang,¹⁹ it seems necessary to take into account the slipping down effect of the LC molecules from the columnar structure due to a large scale fluctuation.

It was reported that a rugged structure exists on the surface of the orientation films.²⁸ In this case, it is sufficient to understand that the symmetry of this rugged surface structure is distorted by performing the rubbing. Then, the occurrence of the pretilt angle and its temperature variation may be argued in the same manner for the simulation which developed in this paper for the branchless polyimide films.

Moreover, in this simulation, we assume that the order parameter is constant over the whole cell region. However, it is commonly said that the surface order parameter is smaller than the bulk order parameter. Then, to carry out this simulation strictly, the spatial variation of the order parameter in the cell must be considered. However, in the present simulation, because we don't need the absolute value of the order parameter but the temperature variation of it, it is considered that the validity of the results is sufficiently kept.

APPENDIX

Expected value of the periodicity induced by the stick slip mechanism.

First, the distance m that the fabric, which is lapped over a cylinder of a rubbing

machine, proceeds during one period of the vibration due to stick slip of each thread is

$$m = \frac{2\pi r R}{60f} \quad (\text{A1})$$

where r , R , f stand for the radius of the cylinder, the rotation rate of the cylinder (r.p.m.), and the frequency of the stick slip.

Next, we evaluate the number of the threads N on the fabric located in the area $p \times q$, where p stands for the diameter of the thread and $q = (2u/v)(2\pi r R/60)$; where v is the velocity of the translating substrate and $2u$ is the contact length of the fabric (see Figure A1); then N is given by

$$N = \frac{4\pi r R D p \sqrt{(r + w)^2 - (r + w - t)^2}}{60v} \quad (\text{A2})$$

where D , w and t stand for the density of the thread ($1/\text{m}^2$), the length of the thread, and the depth of the deformation of the thread by the contact (see Figure A1).

Thus, we are able to calculate the periodicity of the structure ($a + b + c$; see Figure 6):

$$(a + b + c) = \frac{m}{N} = 50 \text{ (nm)}; \quad (\text{A3})$$

in this calculation, the periodicity is assumed to be formed by a successive movement

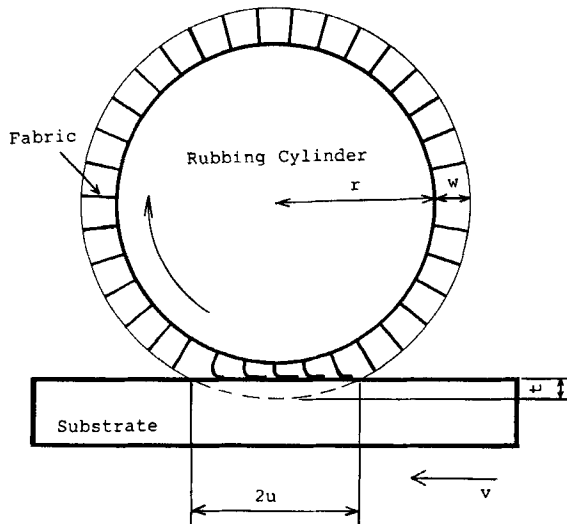


FIGURE A1 An illustrative drawing for the rubbing condition.

TABLE AI

The values used in the calculation for the periodicity of the surface structure

| | | |
|-----|---------------------|----------------------|
| r | (m) | 25×10^{-3} |
| R | (r.p.m.) | 1×10^3 |
| v | (m/s) | 4×10^{-2} |
| t | (m) | 3×10^{-4} |
| w | (m) | 1.5×10^{-3} |
| p | (m) | 5×10^{-6} |
| D | (1/m ²) | 4×10^8 |
| f | (Hz) | 5×10^4 |

of the threads whose number is N , and it was calculated as 50 nm by substituting the values relevant to this problem as tabulated in Table AI.

Acknowledgment

The authors are deeply indebted to Dr. A. Kohno of The Institute of Physical and Chemical Research for his suggestion for evaluating the periodicity formed by the stick slip process as described in the appendix.

References

1. J. Cognard, *Mol. Cryst. Liq. Cryst. Suppl.* **1** (1982).
2. H. Yokoyama, in *Mol. Cryst. Liq. Cryst.*, The 100th Anniversary of Liquid Crystal Research, ed. by S. Kobayashi **165**, 265 (1988).
3. A. Miyaji, M. Yamaguchi, A. Toda, H. Mada and S. Kobayashi, *IEEE. Trans. Electron Devices*, **ED-24**, 811 (1977).
4. T. J. Scheffer and J. Nehring, *Appl. Phys. Lett.*, **45**, 1021 (1984).
5. K. Yoshida, H. Fukuro and S. Kobayashi, *Proc.*, SID **28**, 155 (1987).
6. M. Akatsuka, K. Katoh and K. Sawada, *Proc.*, SID **28**, 159 (1987).
7. M. E. Becker, R. Kilian, B. B. Kosmoski and D. A. Mlynski, *Mol. Cryst. Liq. Cryst.*, **132**, 167 (1986).
8. D. S. Seo, K. Muroi and S. Kobayashi, *Mol. Cryst. Liq. Cryst.*, **213**, 223 (1992).
9. H. Fukuro and S. Kobayashi, *Mol. Cryst. Liq. Cryst.*, **163**, 157 (1988).
10. S. Kuniyasu, H. Fukuro, S. Maeda, K. Nakaya, M. Nitta, N. Ozaki and S. Kobayashi, *Jpn. J. Appl. Phys.*, **27**, 827 (1988).
11. T. Suguyama, S. Kuniyasu, D. S. Seo, H. Fukuro and S. Kobayashi, *Jpn. J. Appl. Phys.*, **29**, 2045 (1990).
12. R. W. Filas and J. S. Patel, *Appl. Phys. Lett.*, **50**, 1426 (1987).
13. S. Matsumoto, M. Kawamoto and K. Kaneko, *Appl. Phys. Lett.*, **27**, 268 (1975).
14. H. Orihara, A. Suzuki, Y. Ishibashi, K. Gouhara, Y. Yamada and N. Yamamoto, *Jpn. J. Appl. Phys.* **L676** (1989).
15. A. Toda, H. Mada and S. Kobayashi, *Jpn. J. Appl. Phys.* **17**, 261 (1978).
16. S. Shimoda, H. Mada and S. Kobayashi, *The Physics and Chemistry of Liquid Crystal Devices*, (G. T. Sprokel ed), Plenum (New York and London, 1981) 47.
17. H. Mada and S. Kobayashi, *Mol. Cryst. Liq. Cryst.*, **53**, 127 (1979).
18. H. Yokoyama, S. Kobayashi and H. Kamei, *J. Appl. Phys.*, **56**, 2645 (1984).
19. H. A. Van Sprang and R. G. Aartsen, *J. Appl. Phys.*, **56**, 251 (1984).
20. F. P. Bowden and L. Leben, *Proc. Roy Soc. London*, **169**, 371 (1939).
21. J. M. Geary, J. W. Googby, A. R. Kmetz and J. S. Patel, *J. Appl. Phys.*, **62**, 4100 (1987).
22. K. Okano, *Jpn. J. Appl. Phys.*, **22**, L343 (1983).
23. T. J. Scheffer and J. Nehring, *J. Appl. Phys.*, **48**, 1783 (1977).

24. D. W. Berreman, *Phys. Rev. Lett.*, **28**, 1683 (1972).
25. G. Vertogen and W. H. de Jeu, *Thermotropic Liquid Crystals, Fundamentals*, eds. Fritz P. Schafer (Springer-Verlag Berlin Heidelberg 1988) Chap. 6.
26. J. Bernasconi, S. Strassler and H. R. Zeller, *Phys. Rev.*, **A22**, 276 (1980).
27. K. Okano *et al.*, *Ekishou Jiten* (Baifuukan, Tokyo, 1989) p. 76 [in Japanese].
28. D. S. Seo, T. Ohide and S. Kobayashi, *Mol. Cryst. Liq. Cryst.*, **214**, 97 (1992).