

Pretilt Angle of Liquid Crystal Related to Anisotropic Polyimide Layer Thickness in a Nematic Liquid Crystal Cell

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ABSTRACT: The property of the unidirectional out-of-plane tilt angle in a nematic liquid crystal is investigated in view of van-der-Waals interaction between nematic liquid crystal molecules and three layers: the anisotropic polyimide layer, the isotropic polyimide layer, and the substrate layer. Dependence of the pretilt angle on the total thickness of the polyimide layer and the thickness of the anisotropic layer

oriented by rubbing is estimated from experiment and theory. Our results show that the screening factor increases with the increase of the thickness of the isotropic layer. © 2006 Wiley Periodicals, Inc. *J Appl Polym Sci* 102: 1505–1508, 2006

Key words: pretilt angle; nematic liquid crystals; LC alignment; surface anchoring

INTRODUCTION

Uniform alignment of liquid crystals (LCs) on an oriented polyimide layer is essential for high quality liquid crystal displays (LCDs). Several methods have been proposed to achieve good alignment.^{1–5} The conventional rubbing technique has many advantages, such as the ease of processing, uniformity, and stability, even though it has some disadvantages, including the electrostatic discharge and the debris by the cloth during the rubbing process. It is still a standard technique for aligning LC molecules in the LCD industry. The out-of-plane tilt angle as well as the in-plane orientation of LCs are very important factors.^{6,7} In optical configurations of LCDs, the pretilt angle is one of the most important parameters because it strongly influences the electro-optical property of various LCD modes including twisted nematic mode,⁸ super-twisted nematic mode,⁹ ferroelectric LC mode,¹⁰ vertical aligned mode,¹¹ and in-plane switching mode.¹² Factors that influence the pretilt angle of LCs have been studied by several scientists. Alexe-Ionescu et al.¹³ reported the measurement of the pretilt angle as a function of the thickness of the polyimide layer. Cnossen et al.¹⁴ reported the measurement of the pretilt angle as a function of the rubbing energy quantified by the thickness of the top layer oriented by rubbing.

Model

In this article, we present the effect of the rubbing energy and the thickness of polyimide layer on the pretilt angle of LCs. Namely, the property of the unidirectional tilt angle of a nematic LC is described in view of van-der-Waals interaction between LC molecules and the three layers: an anisotropic portion of the polyimide layer, an isotropic portion of the polyimide layer, and the substrate layer. The total thickness of a polyimide layer is commonly 80–150 nm. Anisotropic portion of the polyimide layer is oriented by rubbing, whose thickness is 1–30 nm depending on the rubbing strength. The polyimide layer influences LC molecules in contact with the polyimide surface. If the total polyimide thickness is smaller than 20 nm, we need to take into account the interaction with the isotropic substrate layer. We evaluated theoretically the pretilt angle under various thicknesses of the polyimide layer.

Figure 1 shows the schematic presentation of a rubbed alignment layer in contact with a nematic LC and the isotropic substrate. It consists of a nematic LC (medium 1), an anisotropic portion of the polyimide layer with thickness d_1 (medium 2), an isotropic portion of the polyimide layer with thickness d_2 (medium 3), and an isotropic substrate (medium 4). In view of van-der-Waals interactions, the total free energy per unit surface for a uniform nematic orientation is

$$f = f_{14} + f_{13} + f_{12} \quad (1)$$

where f_{14} , f_{13} , and f_{12} are LC-substrate, LC-isotropic polyimide, and LC-anisotropic polyimide interaction,

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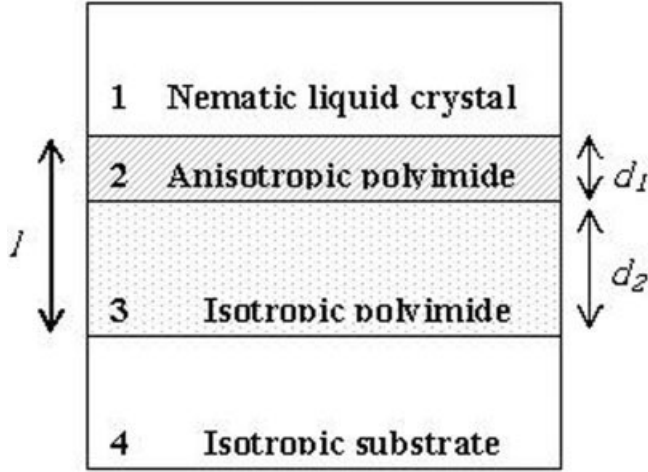


Figure 1 Schematic drawing of an oriented portion of the polyimide layer, an isotropic portion of the polyimide layer, and an isotropic substrate layer.

respectively. Here, we ignored the terms f_{34} , f_{24} , and f_{23} corresponding to isotropic polyimide-substrate, anisotropic polyimide-substrate, and anisotropic-isotropic polyimide interaction, respectively, since LC orientation is expected to be independent of these. f_{14} and f_{13} , which are due to isotropic van-der-Waals-like interactions, can be written in the following forms

$$f_{14} = \frac{1}{2} \frac{A_{14}}{l^{c_1 - c_2(l-d_1)}} \sin^2(\varphi_1 - \varphi_4) \quad (2)$$

$$f_{13} = \frac{1}{2} \frac{A_{13}}{(d_0 + d_1)^{c_1}} \sin^2(\varphi_1 - \varphi_3) \quad (3)$$

where $l = d_1 + d_2$ is the total thickness of the polyimide layer, φ_1 is the average angle of the nematic LC, and φ_3 and φ_4 are easy axes of the isotropic polyimide and the substrate characterizing the 1–3 and 1–4 interactions, respectively. d_0 is the nearest distance between LCs and the surface of the anisotropic layer. A_{13} and A_{14} are connected to the polarizability of LC. $1/\text{day}^{c_1}$ and $1/L^{c_1 - c_2(l-d_1)}$ dependence of the terms f_{13} , f_{14} take into account the screening effect of the polyimide layer. c_1 is not fixed number here unlike in a typical van-der-Waals term where c_1 is fixed as 3. We assumed that the screening effect in the oriented portion of the polyimide is different from that of the isotropic portion. c_1 is a coefficient screened only by the anisotropic layer and $c_1 - c_2(l-d_1)$ is a variable screened by the two layers; the anisotropic layer and the isotropic layer. f_{12} is not screened and has the following form

$$f_{12} = \frac{1}{2} u_{12} \sin^2(\varphi_1 - \varphi_2) \quad (4)$$

where φ_2 is the easy axis of the rubbed polyimide. f_{12} is independent of the thickness at a fixed temperature. As a result, the total free energy is

$$f = \frac{1}{2} v_{14}(l, d_1) \sin^2(\varphi_1 - \varphi_4) + \frac{1}{2} w_{13}(d_1) \sin^2(\varphi_1 - \varphi_3) + \frac{1}{2} u_{12} \sin^2(\varphi_1 - \varphi_2) \quad (5)$$

where

$$v_{14} = \frac{A_{14}}{l^{c_1 - c_2(l-d_1)}}, \quad w_{13} = \frac{A_{13}}{(d_0 + d_1)^{c_1}}.$$

In eq. (5), the interaction with the substrate disappears ($v_4 \approx 0$) for a large total thickness of the polyimide layer. An expression for the pretilt angle φ_1 obtained by minimization of the total surface free energy f with respect to φ_1 is given by

$$\tan(2\varphi_1) = \frac{v_{14}(l, d_1) \sin(2\varphi_4) + w_{13}(d_1) \sin(2\varphi_3) + u_{12} \sin(2\varphi_2)}{v_{14}(l, d_1) \cos(2\varphi_4) + w_{13}(d_1) \cos(2\varphi_3) + u_{12} \cos(2\varphi_2)}. \quad (6)$$

According to this equation, the pretilt angle depends on the thickness d_1 of the oriented layer and the total thickness l of the polyimide layer. The anchoring energy is given by

$$W_{RP} = \frac{d^2 f}{d\varphi_1^2} = [v_{14}(l, d_1) \cos(2\varphi_4) + w_{13}(d_1) \cos(2\varphi_3) + u_{12} \cos(2\varphi_2)] \cos(2\varphi_1) + [v_{14}(l, d_1) \sin(2\varphi_4) + w_{13}(d_1) \sin(2\varphi_3) + u_{12} \sin(2\varphi_2)] \sin(2\varphi_1). \quad (7)$$

from the Rapini-Papoular form. Equation (7) is related to the polar anchoring energy, which is influenced by the thickness of each layer and depends on the relative anchorings of A_{13} , A_{14} , and u_{12} . This theory is evaluated by experimental results and by measuring surface properties related to out-of-plane deviations of the LC director. c_1 and c_2 are constants determined for the polyimides used and the relative anchorings of each layer could be estimated reasonably.

EXPERIMENT AND RESULTS

Materials

Cells are prepared for experiments in the following manner. The glass substrates are spin-coated with a polyimide (SE-3140, Nissan Chemical) and prebaked at 80°C for 10 min and cured at 250°C for 2 hours. Antiparallel cells were filled with a LC (Merck LC

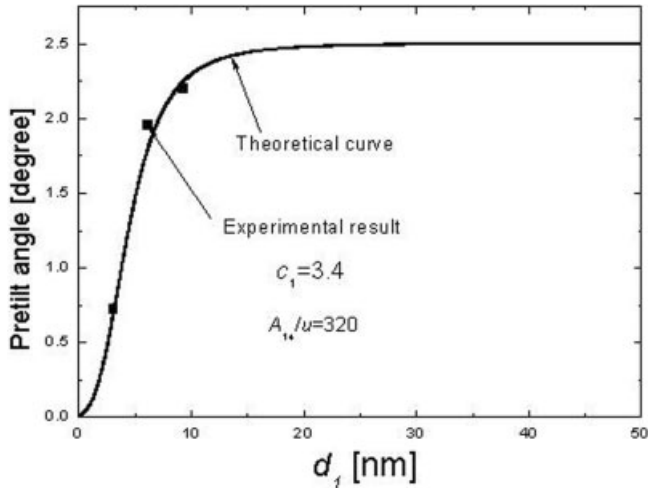


Figure 2 Dependence of the pretilt angle on only the thickness, d_1 , of anisotropic layer (when the thickness of isotropic layer, $d_2 = 0$) with respect to an interaction between substrate and LC.

ZLI-1557) to measure the pretilt angle of LC. The thickness of the polyimide layer was varied by changing the concentration of the polyamic acid solution. The thickness l was measured exactly by an ellipsometer. The thickness of the anisotropic portion, d_1 , was determined by a photoelastic modulator.¹³

Fitting

To determine c_1 , we made all of the polyimide layer to be anisotropic ($d_2 = 0$) by controlling the rubbing strength. Then, we found that, as shown in Figure 2, c_1 and A_{14}/u_{12} are 3.4 and 320 nm³, respectively, which means that the interaction energy of LC molecules with the glass surface is about 320 times stronger than with the anisotropic polyimide. The pretilt angle φ_2 is 4.5° at an infinite thickness of the orientation layer and the glass surface induces a planar anchoring ($\varphi_4 = 0^\circ$). These values agree well with the results of Cnossen et al.¹⁵

Figure 3 is a plot of the pretilt angle of a nematic LC as a function of the thickness of the oriented polyimide layer. The solid line is the best fit obtained from eq. (6) by experiments. $\varphi_3 = 26^\circ$ is determined by the surface second harmonic generation measurement and $l = 10$ nm, $d_0 \sim 1$ nm. Then c_2 and A_{13}/u_{12} were -0.06 and 0.7 nm³, respectively, which means that the interaction energy of LC molecules with isotropic polyimide is about 0.7 times of that with the anisotropic polyimide. This indicates that increase of l increases screening. For $l > 20$ nm, screen factor $c_1 - c_2(l - d_1)$ is greater than 4. If $l \gg 15$ nm, v_{14} could be neglected. For $l > 30$ nm the pretilt angle is independent of the thickness.

Figure 4 shows the relative strength of polar anchoring described as the Rapini-Papoular form of eq. (7)

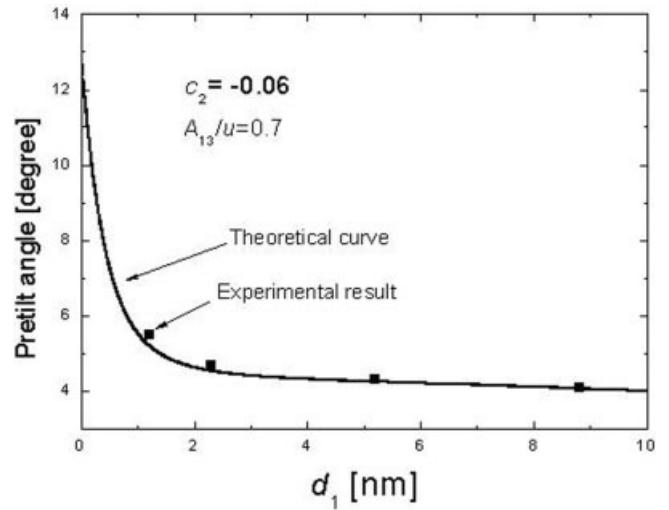


Figure 3 The pretilt angle of a nematic LC as a function of the oriented portion of the polyimide layer, d_1 (when the thickness of isotropic layer, $d_2 \neq 0$) The dot line is measured values and the solid line is the best fit obtained by eq. (6).

for u_{12} . It is nearly constant for $d_1 \cong 30$ nm and then, the polar anchoring strength could be determined only by the interaction u_{12} related to the anisotropic part. For $d_1 \cong 0$ nm, the anchoring strength connected to the isotropic part of the surface is $\sim 1.5 u_{12}$.

CONCLUSIONS

In conclusion $1/d^{c_1}$ and $1/L^{c_1 - c_2(l - d_1)}$ dependence of the terms f_{13}, f_{14} takes into account the screening effect of the polyimide layer. Our results show that c_1 is not fixed number unlike in a typical van-der-Waals term where c_1 is fixed as 3. With increasing l , $c_1 - c_2(l - d_1)$ increases gradually and the screening effect depends

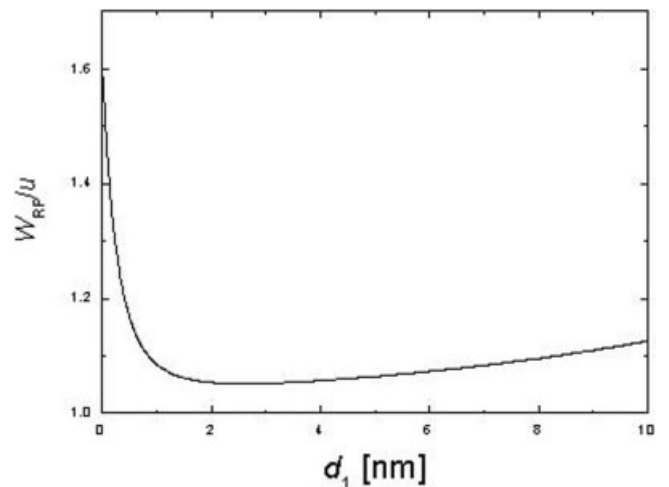


Figure 4 The relative strength of polar anchoring as a function of d_1 described in the Rapini-Papoular form for u_{12} .

on the thickness of the isotropic and the anisotropic layer. The theoretical model agrees well with the experimental results.

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