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NUMERICAL CALCULATIONS OF ELECTROCLINIC EFFECT: EFFECT OF THE POLAR ANCHORING STRENGTH

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Abstract Numerical calculations of the electroclinic effect in the smectic-A phase, which is based on the Landau-type free energy formula, are performed. Experimentally, the deviation of the bulk LC director from the rubbing direction has been observed. Our numerical calculation of the molecular alignment can explain this phenomenon by considering the influence of the polar surface anchoring on the LC molecular orientational distribution.

1 Introduction

The electroclinic effect (ECE) in the smectic phase of chiral liquid crystal (LC) is known for the molecular tilting phenomenon and accompanied critical behavior.[1] When an electric field is applied parallel to the smectic layer, field-induced molecular tilt can be observed, where the tilt angle depends on the magnitude of the applied field. Particularly, the response speed are excellently fast because of the soft mode response, which is much attractive capability for the flat panel display devices. Nowadays, ECE was studied by many researchers from the experimental and the theoretical point of view.

Recently, the dynamic simulation of ECE phenomena, which was based on the Landau-type free energy formula, was proposed.[2] In this simulation, the surface anchoring effect, the elastic effect and the polarization electric field were also taken into account. It was found that the dynamic response of the dielectric constant depends on the order of the phase transition. This numerical

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examination agreed with out experimental results qualitatively. Furthermore our numerical results also showed the remarkable effect of the non-polar and/or polar surface anchoring strength on the molecular dynamic reorientation.

Experimentally, it was found that in the smectic-A phase the bulk LC director and hence the smectic layer normal deviates from the rubbing direction by an angle θ.[3, 4] J. Xue *et. al.*[5] and W. Chen *et. al.*[6] studied this phenomenon as the surface ECE. In order to discuss the temperature dependence of θ, they introduced the Landau-type free energy formula, where the surface polar anchoring energy was also considered. The polar anchoring was assumed to be originated from interaction of the LC molecules with a local electric field at the boundary. However, in order to make this discussion simple, higher order terms in the Landau-type free energy formula was neglected, and the orientational distribution of the LC molecules throughout the cell and the magnitude of the polar anchoring strength were not clarified.

In the present work, the detailed numerical calculation of the molecular orientational distribution is studied. The comparison between the numerical and the experimental results and the estimation for the order of the polar anchoring strength are also discussed.

2 Theoretical model

The details of this theoretical equations for ECE calculations have been published.[2] It is well known that the ECE can be understood by analyzing the Landau-type free energy formula,[1, 7, 8, 9]

$$\begin{aligned} f_{\mathrm{Landau}} &= f_0 + \frac{1}{2}A\theta^2 + \frac{1}{4}B\theta^4 + \frac{1}{6}C\theta^6 + \frac{1}{2}\chi_{\mathrm{p}}^{-1}P^2 \\ &\quad - \frac{1}{2}(\epsilon^0 + \epsilon^1\theta^2)E_Y^2 - PE_Y - c\,\theta P, \end{aligned} \tag{1}$$

where P is the component of the average polarization due to the orientation of permanent dipoles parallel to the applied electric field E_Y. The polarization P and molecular tilt angle θ are treated as independent variables. ϵ^0 is the conventional dielectric constant without contribution from the permanent dipole, ϵ^1 is the coefficient of the dielectric energy term corresponding to the field-induced dielectric biaxiality. χ_{p} is a generalized susceptibility, and c is the piezoelectric coupling constant. $A = a(T - T_0)$, B and C are the Landau coefficient. E_Y is given by

$$E_Y = -\frac{d\phi}{dY} = -\phi_{,Y}, \tag{2}$$

where ϕ is the electric scalar potential. The elastic free energy density f_{elas}, which is conventionally used in the elastic deformation, is simply given by

$$f_{\mathrm{elas}} = \frac{1}{2}K(\frac{d\theta}{dY})^2, \tag{3}$$

where K is the elastic constant.

We assume that the surfaces of bounding plates are homogeneous and characterized by the surface anchoring energy per unit area f_s given by[7]

$$f_s^d = U\theta_d + \frac{1}{2}G\theta_d^2, \tag{4}$$

where superscripts d indicates the value at the upper boundary plate. The first term represents polar anchoring energy, which have a correlation to the interaction between the LC molecule and alignment surface. The second term represents non-polar and in-plane tilt (azimuthal) anchoring energy. In this study, the lower boundary plate is supposed to be free surface, which corresponds to the surface alignment with non-rubbed treatment.

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

$$F = \int_0^d (f_{\mathrm{Landau}} + f_{\mathrm{elas}} + f_S^d \delta(Y - d))dY. \tag{5}$$

For minimizing the total free energy, we resort to the conventional difference method for the space Y derivatives. The scalar potential ϕ is also calculated simultaneously, which is determined from $\delta F/\delta\phi=0$.

Then we can calculate the molecular orientational distribution throughout the cell. The number of divisions along the $Y-$axis is 40. The used parameters used in our calculations, which are based on those of the LC (R)-4-(1-trifluoromethylheptyloxy-carbonyl)- phenyl 4-(5-dodecyloxypyrimidin-2-yl) benzoate[10] (TFMHPDOPB), are as follows. Landau coefficient $A = 8 \times 10^4$ ($\mathrm{Jm^{-3}K^{-1}rad^{-2}}$), $B = -1\times10^6$ ($\mathrm{Jm^{-3}K^{-1}rad^{-4}}$) and $C = 6\times10^6$ ($\mathrm{Jm^{-3}K^{-1}rad^{-6}}$). The generalized susceptibility $\chi_p = 1 \times 10^{-10}$ (F/m), the piezoelectric coupling constant $c = 5.6 \times 10^7$ (V/m), elastic constant $K = 1.0 \times 10^{-10}$ (N), and the conventional dielectric coefficient $\varepsilon^0 = 5 \times 10^{-11}$ (F/m). Here, the dielectric biaxiality ε^1 was neglected. Because the principal origin of the ECE is not the electronic polarization, but the polarization P due to the orientation of the permanent dipoles, the effect of dielectric biaxiality seems to be small. The cell thickness assumed to be d=2 (μm). In this calculation, external electric field was supposed to be not applied.

3 Experimental

The LC materials used were TFMHPDOPB.[10] (Mitsubishi Chemical Co., Ltd.) and 764E (Merck. Ltd.) The structure of the cell was of the ordinary homogeneous type. The cell consisted of two glass plates whose inner surface were coated with polyimide (PI), and only one side PI surface of the sample cell was pre-rubbed. The magnitude of rubbing strength was carefully controlled. Thickness of the sample cell was about 2μm. After filling the LC at the isotropic temperature, the cell was cooled down with the temperature gradient so that the smectic layer grew from the rubbed substrate.[11, 6] In order to investigate the effect of surface-alignment PI films, we prepared three types of PI; PI-1, PI-4[12] (Japan Synthetic Rubber Co., Ltd.) and PIX-5400 (Hitachi Chemical Co., Ltd.).

4 Reesults and Discussions

Figure 1 shows the numerical results of the molecular orientational distribution throughout the cell. In these calculations, the surface anchoring strength at the upper boundary surface is supposed that the non-polar anchoring strength $G=1\times10^{-4}$ (J/m^2), and the polar anchoring strength U ranged from 1×10^{-4} (J/m^2) to 1×10^{-3} (J/m^2). Especially, the LC molecule at the upper boundary is supposed to be aligned parallel to the rubbing direction, which is grounded on the experimental result of the measurement of second harmonic generations (SHG)[6]. The lower surface is assumed to be free surface (not anchored), because the lower substrate of the LC sample experimentally used is not rubbed. It is found that the distortion of the molecular orientation tends to localize near the upper boundary surface, and the orientational distribution from the bulk to the lower boundary surface is almost uniform. That is, even the molecule at the upper boundary surface is aligned parallel to the rubbing direction, the bulk LC molecules deviate from the rubbing direction. The model of this orientation is illustrated in Figure 2.

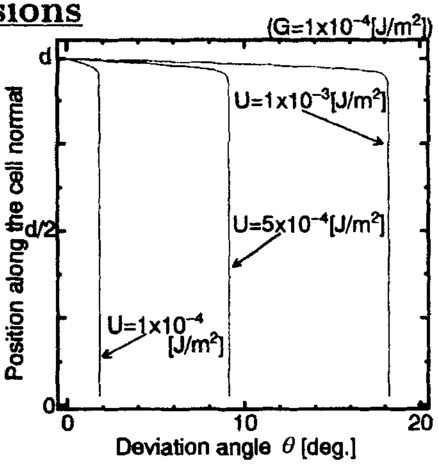

Figure 1 Numerical results of the molecular orientational distribution.

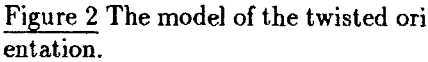

Figure 2 The model of the twisted orientation.

It is also found that the deviation angle depends on the polar anchoring strength. The dependence of the deviation angle on the polar anchoring strength are shown in Figure 3, where the non-polar anchoring strength ranged from 5×10^{-3} (J/m^2) to 1×10^{-5} (J/m^2) as the parameter. The dependence of the deviation angle on the non-polar anchoring strength are also shown in Figure 4,

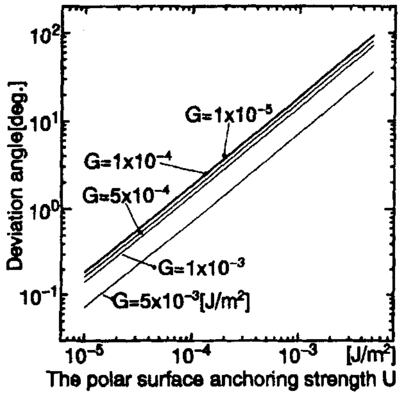

Figure 3 The dependence of the deviation angle on the polar anchoring strength.

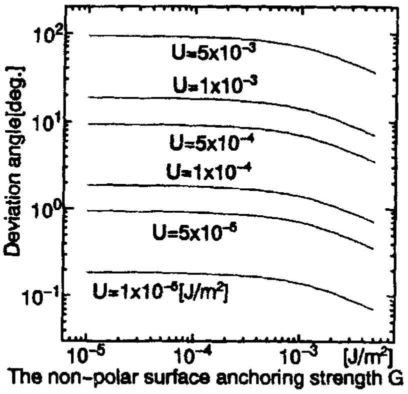

Figure 4 The dependence of the deviation angle on the non-polar anchoring strength.

where the polar anchoring strength ranged from 5×10^{-3} (J/m^2) to 1×10^{-5} (J/m^2) as the parameter. From these numerical results, not only the polar anchoring strength but also the non-polar anchoring strength remarkably effect on the deviation angle of the bulk LC molecule from the rubbing direction.

Figure 5 shows the microphotograph of the LC sample cell in the smectic A phase under the crossed polarizers, where the LC and PI used were TFMH-PDOPB and PI-1, respectively. The rubbing direction, crossed polarizers and extinction angle are indicated by arrows. The director in the bulk is identical with the extinction angle. It is found that the director in the bulk deviates from the rubbing direction, this deviation is as large as 20.3°. The director distribution seems to correspond with the model illustrated in Fig. 2. Comparing with the numerical result shown in Fig. 3, the polar anchoring strength may be the order of 10^{-4}(J/m^2), provided that the non-polar anchoring strength is 1×10^{-4}(J/m^2). This result suggests that the polar anchoring strength is not so small that it can be ignored.

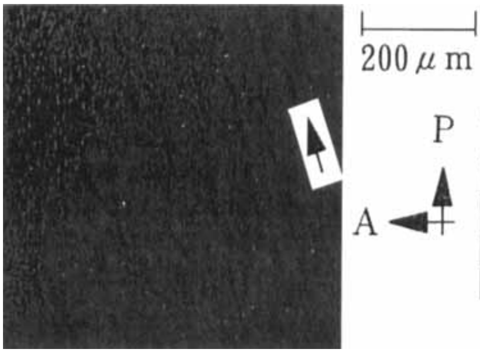

Table 1 Deviation angle dependence on PI and LC.

	TFMHPDOPB	764E
PI-1	20.3°	17.3°
PI-4	6.0°	7.7°
PIX-5400	15.7°	12.6°

Figure 5 Microphotograph of the sample cell whose director in the bulk was deviated from the rubbing direction. (See Color Plate I).

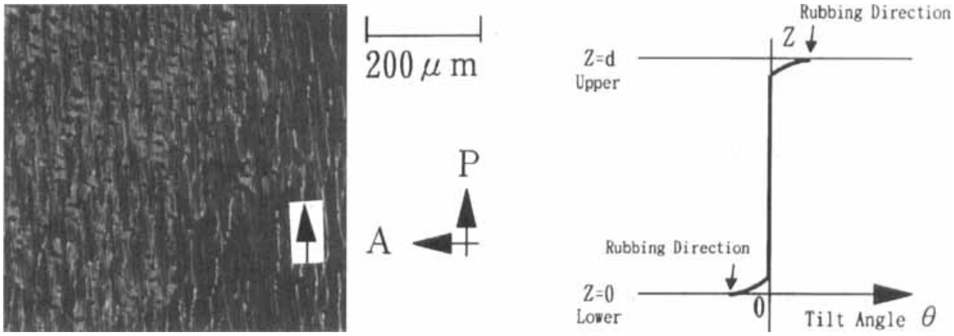

Figure 6 Microphotograph and orientational model of the intersected rubbing cell. (See Color Plate II).

The results of the deviations for the other samples was also shown in Table 1. From this result, it is found that the deviation angle tends to depend on the alignment polyimide film in both LC materials.

Figure 6 is the polarized optical microscopic texture of the sandwich cell in the smectic A phase, the LC and PI used were TFMHPDOPB and PI-1. In particular, both of the upper and the lower substrates were pre-rubbed, where the rubbing directions were arranged to be intersected each other, *i. e.*, the intersecting angle is two times of the deviation angle. It is found that the extinction angle is just in the middle between the two rubbing direction. The simple model of the twisted orientational distribution is also shown in Fig. 6. From this experimental result, the director in the bulk may be controlled exactly by this intersected rubbing.

In the case of the surface stabilized ferroelectric liquid crystal (SSFLC) cell, it has been described that the half spray (twisted) orientation appears when the polar anchoring exists.[13] To avoid the effect of the polar anchoring, it was reported that the intersected rubbing treatment is much effective to form the uniform texture.[14] This series of studies may give an explanation why the intersected rubbing treatment is much effective for SSFLC cell and may predict the suitable angle for intersected rubbing.

5 Conclusion

The effect of the polar anchoring strength on the orientational distribution throughout the cell were investigated by means of numerical calculations based on the Landau-type free energy equation. The numerical results demonstrated a remarkable effect of the non-polar and/or polar surface anchoring strength on the molecular orientation. Our experimental results were also compared with these calculations. It is proposed that the polar anchoring strength is not so small that it can be ignored. This series of studies may give an explanation why the intersected rubbing treatment is much effective for SSFLC cell and may predict the suitable angle for intersected rubbing. Detailed researches on the effect of the surface effect and phase transition behaviors are now in progress and will be presented in the near future.

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