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Effect of the Surface Anchoring Energy on Modeling the Defect in the Liquid Crystal Director Field

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In this research, we studied the effect of the surface anchoring energy on the defect modeling in the liquid crystal (LC) director field. In order to model the defect of a LC cell, we make use of the fast Q-tensor method, in which the scalar order parameter S and the orientation of the LC director at each gird point of the LC cell can be calculated. The modeling of the defect generation was performed by using the "pincement" of Bouligrand, which shows a reverse tilt-wall and a pair of defect nucleations. We carefully inspected the position of the defect generation in the LC cell as a function of the surface anchoring energy. By using the fast Q-tensor method to consider the tensor form of the surface anchoring energy, we could model both the LC orientation and the generated defect more precisely.

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I. INTRODUCTION

Liquid Crystals (LCs) have been widely used for applications including display devices and optical components for communication because of the excellent electro-optical characteristics, fast response, and wide viewing angle. The advantages of liquid crystal displays (LCDs) are achieved by using various LC modes such as pi-cell [1], multi-domain cell, patterned vertically aligned cell [2] and fringe field switching cell [3] modes, which can enhance the electro-optic characteristics. Generally, these LC modes use the multi-domain technology in a single pixel for excellent viewing angle, so they suffer from a nonuniform voltage distribution in a single pixel due to the multi-domain effect. This may induce the storage of a very high elastic energy in a very small area. Therefore, this multi-domain effect can induce a spatial area with a scalar order parameter $S = 0$ (defect area) when a voltage is applied to the pixel. In general, the defects generated in the LCD mode can strongly influence the optical properties, such as the transmittance, response time, and viewing angle. Therefore, an understanding of the defect dynamics in the LC director field has become more important for the advanced LC modes.

In order to achieve the equilibrium state of an LC director configuration with a defect, we need to calculate the Gibb's free energy of the LC director field [4]. In general, the Gibb's free energy consists of elastic deformation terms and electric field terms. One of the representative expressions of the Gibb's free energy is the vector form of the Oseen-Frank equation, which uses three elastic constants (splay, twist and bend). The vector method of the Oseen-Frank equation, however, treats the scalar order parameter as a constant 1 at all LC grid points, so it cannot handle the defect dynamics. Another method to calculate the equilibrium state of the LC director configuration is to use the Q-tensor representation of de Gennes. This method can calculate the defect dynamics and the phase transition between topologically inequivalent states of the LC director field by applying a thermal energy term. However, in this approach, the tensor representation needs to be expanded to third order in order to remove the degeneracy between the bend and the splay elastic constants of the LC cell, so a very complicate process for the calculation is required [5].

Also, Dickman *et al.* have proven that if we use only one third-order component, the Oseen - Frank vector representation can go directly to the Q-tensor representation [6]. Therefore, Dickman *et al.* could provide a qualitative analysis for the phase transition between the topologically inequivalent state and the LC director field with a defect, but not a quantitative result, because they did not consider the calculation of the scalar order parame-

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ter in the LC grids. In previous papers, the fast Q-tensor method, which can provide qualitative and quantitative calculations of the LC director field with a defect by applying a temperature energy term to the strain energy term of the Dickman's tensor form, has been proposed [7-9].

In this paper, we study the effect of the surface anchoring energy, which is based on the *Rapinni - Papoular* equation, in order to model the generation of the defect in the LC director field precisely. First of all, we apply the tensor form of the *Rapinni - Papoular* equation to the total free energy for modeling the LC director. Then, we calculate the LC orientation and the scalar order parameter S in each LC grid. Modeling of the LC director field was performed by using the "pincement" of Bouligrand, which shows a reverse tilt-wall. For this, we carefully inspect the difference between the modeled LC director field when applying a strong anchoring energy and a weak anchoring energy.

II. FAST Q-TENSOR METHOD WITH SURFACE ANCHORING ENERGY

The fast Q-tensor method uses an elastic energy term, an electric energy term and a temperature energy term as below [7-9]:

$$\begin{aligned} f_s &= \frac{1}{12}(K_{33}-D_{11}+3K_{22})\frac{G_1^{(2)}}{S^2} \\ &+\frac{1}{2}(K_{11}-K_{22}-3K_{24})\frac{G_2^{(2)}}{S^2}+\frac{1}{2}K_{24}\frac{G_3^{(2)}}{S^2} \\ &+\frac{1}{6}(K_{33}-K_{11})\frac{G_6^{(2)}}{S^3}+q_0K_{22}\frac{G_4^{(2)}}{S^2}, \qquad (1) \\ G_1^{(2)} &= Q_{jk,l}Q_{jk,l}, \quad G_2^{(2)}=Q_{jk,k}Q_{jl,l}, \\ G_3^{(2)} &= Q_{jk,l}Q_{jl,k}, \quad G_4^{(2)}=e_{jkl}Q_{jm}Q_{jm,l}, \\ G_6^{(2)} &= Q_{jk}Q_{lm,j}Q_{lm,k}, \\ Q_{jk} &= S\left(n_jn_k-\frac{\delta_{jk}}{3}\right), \quad Q_{jk,l}=\frac{\partial Q_{jk}}{\partial l}, \end{aligned}$$

where K_{11}, K_{22}, and K_{33} are the splay, twist and bend constants, respectively. K_{24} is associated with the surface anchoring energy. If we assume that the LC directors are fixed at the surface layer, K_{24} can be ignored. The q_0 is the LC chirality. The Levi-Civita symbol e_{ijk} is 1 when subscripts are in the order of xyz, yzx, or zxy, is -1 when the subscript order is xzy, yxz, or zyx, and is 0 otherwise. The δ_{jk} is the Kronecker delta, which is 1 if j equals k, and is 0 otherwise.

The Q-tensor representation of the electric energy term is directly derived from $f_e = D\cdot E/2$ as

$$\begin{aligned} f_e &= \frac{1}{2}\varepsilon_0\left(\bar{\varepsilon}V_{,j}^2+\Delta\varepsilon V_{,j}V_{,k}\frac{Q_{jk}}{S}\right), \qquad (2) \\ \bar{\varepsilon} &= \frac{2\varepsilon_\perp+\varepsilon_\Pi}{3}, \quad \Delta\varepsilon=\varepsilon_\perp-\varepsilon_\Pi, \quad V_{,j}=\frac{\partial V}{\partial j}. \end{aligned}$$

The Q-tensor is not written in a vector notation as shown in Eq. (1) and in its definition. Therefore, we can assume that the LC director never has a different energy state due to the sign of the neighboring directors, so we can avoid the failure of LC modeling caused by vector notation. In spite of this merit, this method cannot model the dynamic LC configuration with defects because it always has a constant order parameter $S = 1$, so to calculate the order parameter S in each grid, we add the temperature, in the absence of a director field distortion, to the Dickman Q-tensor representation [7-9]. A temperature energy term determines the order parameter S as a function of temperature because the order parameter S is directly associated with the temperature. The tensor formulation of the temperature energy can be simply described by using the following polynomial expansion:

$$\begin{aligned} f_t(T) &= f_0+\frac{1}{2}A(T)Q_{ij}Q_{ji}+\frac{1}{3}B(T)Q_{ij}Q_{jk}Q_{ki} \\ &+\frac{1}{4}C(T)(Q_{ij}Q_{ij})^2+O(Q^5). \qquad (3) \end{aligned}$$

By applying thermal energy to the total free energy, we expect the director modeling in regard to both the LC orientation and the defect in the LC layer to be exact. In this paper, we apply the surface anchoring energy term, in addition to the elastic, electric and temperature term, in order to achieve a more exact LC director field configuration and order parameter S in a LC cell because the surface anchoring energy can cause a serious change in the energy state in the bulk area. The tensor representation of the surface anchoring energy based on the *Rapinni - Papoular* equation is [10]

$$f_{surface} = \frac{1}{2}W(Q_{ij}-Q'_{ij})^2, \qquad (4)$$

where W is a constant related to the anchoring strength. Q_{ij} and Q'_{ij} are tensor order parameters with strong and weak anchoring strength corresponding to the easy axis, respectively. Therefore, the total Gibb's free energy can be summarized as the sum of Eqs. (1), (2), (3), and (4). In order to achieve the equilibrium state of the LC director configuration at constant applied potential, we use the Euler-Lagrange equation, which is $0 = -[f_g]_{Q_{jk}}$ and $0 = -[f_g]_V = \nabla\cdot D$, where $[f_g]_{Q_{jk}}$ and $[f_g]_V$ represent the functional derivatives of the energy density with respect to Q_{jk} and voltage V. By using these equations, we can calculate the components of the 3-by-3 Q-tensor and voltage in each grid. The expressions of the functional derivatives for each energy term are as follows:

$$\begin{aligned} [f_g]_{Q_{jk}} &= \text{strain term}([f_g]_S)+\text{voltage term}([f_g]_V) \\ &+\text{temperature term}([f_g]_T) \\ &+\text{surface anchoring term}([f_g]_{Sur}), \\ [f_g]_S &= -2\left(-\frac{1}{12}K_{11}+\frac{1}{4}K_{22}+\frac{1}{12}K_{33}\right)Q_{jk,ll} \\ &-(K_{11}-K_{22}-K_{33})Q_{jl,lk}-K_{24}Q_{jl,lk} \qquad (5) \\ &+\frac{1}{4}(K_{33}-K_{11})(Q_{lm,j}Q_{lm,k}-Q_{lm,l}Q_{jk,m} \end{aligned}$$

$$
\begin{aligned}
& -Q_{lm}Q_{jk,ml} - Q_{lm,m}Q_{jk,l} - Q_{lm}Q_{jk,lm}) \\
& +2q_0K_{22}e_{jlm}Q_{mk,l}, \\
[f_g]_V &= -\frac{1}{2}e_0D_eV_{,j}V_{,k}, \\
[f_g]_T &= \left(A_1 + A_2\frac{T}{T_{ni}}\right)Q \cdot Q + A_3Q \cdot Q \cdot Q \\
& +A_4Q \cdot Q \cdot Q \cdot Q, \\
[f_g]_{Sur} &= W(Q'_{jk} - Q_{jk}), \\
Q_{jk,ll} &= \frac{\partial}{\partial l}\left(\frac{\partial Q_{jk}}{\partial l}\right),
\end{aligned}
$$

where T is the current temperature, T_{ni} is the nematic-isotropic transition temperature and the constants from A_1 to A_4 represent the thermal coefficients for the fitting polynomial. Constants depend on the nematic LC material properties. To find the values of the coefficients, we need to try to fit the order parameter S and calculated T_{ni} to the experiment data ($S = 0.6$ at 25 °C, T_{ni} = 95 °C) [7-9]. The calculated values of each coefficient from A_1 to A_4 are 0.79, 0.794, 0.61, and 1.474 J/cm^3, respectively.

The dynamic equation $\gamma(\partial Q_{jk}/\partial t) = -[f_g]_{Q_{jk}}$ is used to achieve the equilibrium state, and γ is the rotational viscosity. The relaxation method based on the dynamic equation for numerical calculation can provide the formulated relation between the Q-tensor of the next time $Q_{jk}^{-\tau+1}$ and that of the current time $Q_{jk}^{-\tau}$:

$$Q_{jk}^{-\tau+1} = Q_{jk}^{-\tau} + \Delta t[f_g]Q_{jk}/\gamma. \tag{6}$$

By using Eq. (7), one can achieve the equilibrium state by iterating the dynamical calculation until the Q-tensor values of the LC director in each grid are saturated. The order parameter S is directly related to the Q-tensor by the equation $S^2 = 1.5(Q \cdot Q)$.

III. SIMULATION OF THE EFFECT OF SURFACE ANCHORING STRENGTH ON DEFECT MODELING

In a previous paper, we modeled the defect in the LC director field through a pincement that showed a reverse tilt wall [7-9]. However, the calculated result of the previous paper could not clear up the origination and the dynamics of the generated defect because the applied strong surface anchoring did not permit exact modeling of the origin of the defect. Pincement is defined as the transformed defect from the wall to a line as shown in Fig. 1 [11]. Figure 1(a) shows the typical reverse tilt wall in the LC cell. The solid line in the cell represents the LC director field. If we apply an outer force, such as an electric or magnetic field, to the cell, the distortion of the LC director field becomes larger. Then, a pair of defects, which have strengths $m = \pm 1/2$, appears in the LC director field, as shown in Fig. 1(b). De Gennes predicted that at some voltage a transition should occur in

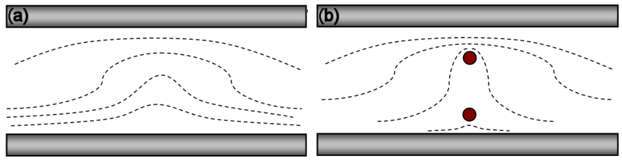

Fig. 1. Illustration of pincement in the LC director field: (a) a reverse tilt wall and (b) a pair of line defects.

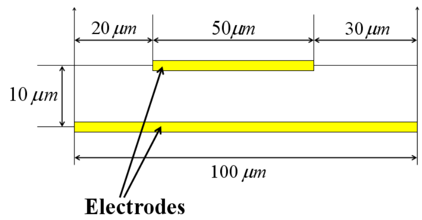

Fig. 2. Cell structure used for the simulation.

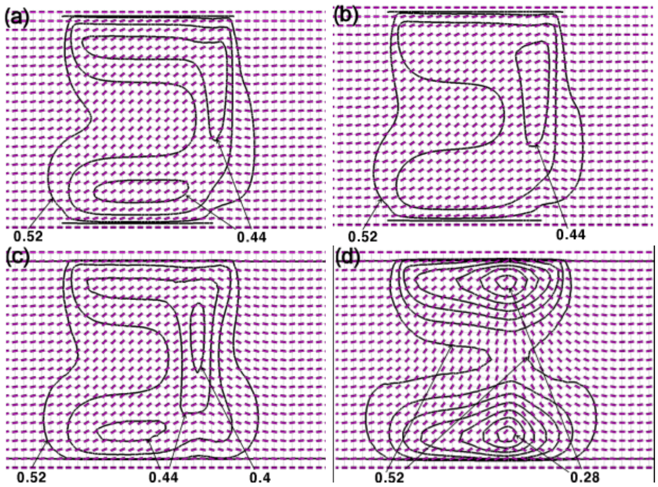

Fig. 3. (Color online) Simulated results using a fast Q-tensor method with strong anchoring strength: (a) at 1.53 V, (b) at 1.55 V, (c) at 1.6 V, and (d) at 1.8 V. The solid lines represent contour lines for the equi-order parameter S.

the middle layer of the LC cell. In order to observe the defect core in the LC director configuration, we should make use of an enormous number of grids because the generated defect core has a molecular dimension. This can require a very long calculation time. To solve this problem, we suggested a numerical approach that applied the values of $A_1 - A_4$ that were 0.01 times their real values instead of the real values of $A_1 - A_4$ [7-9]. This permits visible observation of the generated defects within a short calculation time. On the contrary, the region of the defect size will be much larger than could actually occur.

For modeling of the pincement, we applied a two-dimentional patterned structure that had a 10-um cell gap and was filled with the LC material ZLI-1565 (k_{11} = 14.4 pN, k_{22} = 6.9 pN, K_{33} = 18.3 pN, $\varepsilon_\perp$ = 3.7, $\varepsilon_\parallel$ = 10.7, and $\Delta\varepsilon$ = 7) for the calculation, as shown in Fig

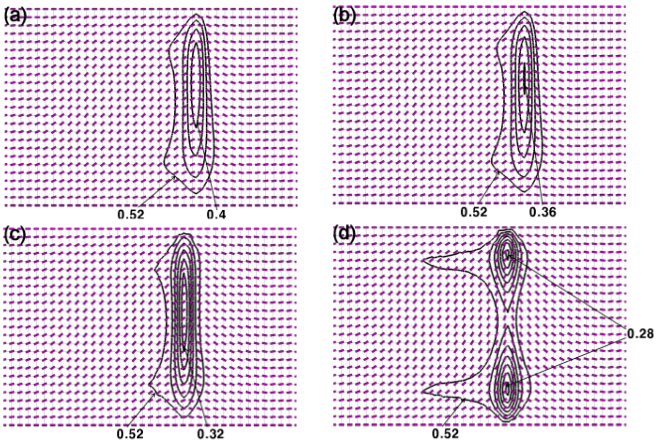

Fig. 4. (Color online) Simulated results using a fast Q-tensor method with weak anchoring strength: (a) at 1.53 V, (b) at 1.55 V, (c) at 1.6 V and (d) at 1.8 V. The solid lines represent contour lines for the equi-order parameter S.

2. We divided the LC layers into 50- by-50 along the x and the z axes for modeling. Figure 3 shows the results calculated using fast Q-tensor method with strong anchoring strength ($W = 1 \times 10^{-3}$ N/m) as a function of the applied voltage. In Fig. 3, solid lines in the cell represent the contour lines for an equi-scalar order parameter, so we can observe the ordering strength in each grid. In the simulation, we found the variation of the scalar order parameter in the LC cell at 1.53 V. As we increase the applied voltage, we can observe the separation of the defect set to the each surface at 1.8 V. From the calculation, we can obviously confirm that a defect pair can be generated in the cell by applying a voltage that sharpens the reverse tilt wall and that moves it to the surface, as shown in Fig. 1(b). On the contrary, the exact position where the defect generated in the LC cell originates is not clear because the calculated order parameter near the surface becomes higher as we increase the applied voltage due to the strong anchoring energy. This may disturb the observation of the nucleation of the generated defect. Therefore, the application of a strong surface anchoring energy should be avoided in modeling the defect dynamics.

Figure 4 shows the calculated result for modeling the defect under the same calculation conditions as those in Fig. 3 when we apply a weak surface anchoring energy ($W = 1 \times 10^{-5}$ N/m). From Fig. 4, we can clearly observe the originating position of the defect from the reverse tilt wall. At 1.53 V, the defect is nucleated at the middle position of the LC layer, and the defect pair is separated to the surface by increasing the voltage. This modeling result coincides exactly with in the description of the pincement as shown in Fig. 1 and in the de Genne's prediction. Therefore, we can confirm that anchoring energy should be considered in order to achieve exact modeling of the generated defect, in addition to the LC orientation in the LC cell.

IV. CONCLUSION

In this research, we studied the effect of the surface anchoring energy on modeling the defect in the LC director field by using the fast Q-tensor method. In order to get exact results in regard to the generated position and strength of the order parameter, we needed to consider an appropriate value of the anchoring energy, instead of the ideal strong anchoring energy, because the defect due to the hard anchoring energy could disappear at the surface. Therefore, the real defect in the LC cell could be filtered from the surface area. As a result, we could model the position and the dynamical behavior of the defect in a LC cell containing a reverse tilt wall more exactly by applying a weak anchoring energy to the surface. This result may help in analyzing the dynamics of the LC director for an advanced LC mode applying the multi-domain effect.

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