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

Wan-Seok Kang, Woo-Yong Joo, Seung-Yeol Hur, Hak-Yong Han, Gi-Dong Lee and Bongsik Jeong*

Department of Electronics Engineering, Dong-A University, Busan 604-714

Hyung-Jin Youn
Sanayi System Co., Ltd., Incheon 402-711, Korea

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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 grid 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 parameter.
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 Rapini - 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 Rapini - Papoular equation to the total free energy for modeling the LC director. Then, we calculate the LC orientation and the scalar or-tor 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].

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]:

\[ f_s = \frac{1}{12} \left[ (K_{11} - D_{11} + 3K_{22}) G_{12}^2 + \frac{1}{2} (K_{22} - K_{11} - 3K_{24}) G_{22}^2 + \frac{1}{2} K_{24} G_{22}^2 \right] \]

\[ + \frac{1}{6} (K_{23} - K_{11}) G_{13}^2 + g_0 (K - K_{22}) G_{13}^2, \]

\[ G_{ij}^{(2)} = Q_{jk,l} Q_{jk,l}, \quad G_{ij}^{(2)} = Q_{jk,l} Q_{jk,l}, \quad G_{ij}^{(2)} = \epsilon_{ijk} Q_{jm} Q_{jm}, \quad \]

\[ Q_{jk} = \left( n_j n_k - \frac{\delta_{jk}}{3} \right), \quad \frac{\partial Q_{jk}}{\partial l} = \frac{\partial Q_{jk}}{\partial l}, \]

where \( K_{11}, K_{22}, \) and \( K_{23} \) 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 \( g_0 \) is the LC chirality. The Levi-Civita symbol \( \epsilon_{ijk} \) is 1 when subscripts are in the order of \( xyz, yxz, \) or \( zyx, \) is -1 when the subscript order is \( zyx, yxz, \) or \( zyx, \) and is 0 otherwise. The \( \delta_{jk} \) is the Kronecker delta, which is 1 if \( j = k, \) and is 0 otherwise.

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

\[ f_e = \frac{1}{\varepsilon_0} \left( \varepsilon V_j^2 + \Delta \varepsilon V_j V_k \frac{Q_{jk}}{S} \right), \]

\[ \varepsilon = \frac{2\varepsilon_0 + \varepsilon_\|}{3}, \quad \Delta \varepsilon = \varepsilon_\perp - \varepsilon_\|, \quad V_j = \frac{\partial V}{\partial j}. \]

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:

\[ f_T(T) = f_0 + \frac{1}{2} A(T) Q_{ij} Q_{ij} + \frac{1}{3} B(T) Q_{ij} Q_{jk} Q_{ki} \]

\[ + \frac{1}{4} C(T) (Q_{ij} Q_{ij})^2 + O(Q^4). \]

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 Rapini - Papoular equation is [10]

\[ f_{surface} = \frac{1}{2} W (Q_{ij} - Q_{ij}')^2, \]

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 \( 0 = -\partial g_0 S_{\alpha} \) and \( 0 = \partial g_0 V = \nabla \cdot D, \) where \( \partial g_0 S_{\alpha} \) and \( \partial g_0 V \) 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:

\[ [f_0] Q_{jk} = \text{strain term}([f_0] s) + \text{voltage term}([f_0] v) \]

\[ + \text{temperature term}([f_0] T) \]

\[ + \text{surface anchoring term}([f_0] S_{\alpha}), \]

\[ [f_0] S = -2 \left( -\frac{1}{12} K_{11} + \frac{1}{4} K_{22} + \frac{1}{12} K_{33} \right) Q_{jk,l,l} \]

\[ - (K_{11} - K_{22} - K_{33}) Q_{jl,l,k} - K_{24} Q_{jl,l,k} \]

\[ + \frac{1}{4} (K_{33} - K_{11}) (Q_{lm,j} Q_{lm,k} - Q_{lm,l} Q_{jk,m}). \]
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 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 \( A_1 \) to \( A_4 \) 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-dimensional 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, \( \epsilon_\perp = 3.7, \epsilon_\parallel = 10.7 \), and \( \Delta \epsilon = 7 \)) for the calculation, as shown in Fig.
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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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REFERENCES