

# Modeling of Defects Nucleation in the Inhomogeneous Liquid Crystal Director Field

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With the fast Q-tensor method, which can model the defect dynamics in a liquid crystal director field, the nucleation and dynamical behavior of defects is modeled. In order to model the defect, homeotropic aligned liquid crystal cell with step inhomogeneous electrode which has a height of 1  $\mu\text{m}$  is used. From the simulation, we can observe the nucleation and line of the defect from surface inhomogeneity and the experiment is performed for confirmation. The experimental result is compared with numerical modeling in order to verify the simulation of the defect nucleation.

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## I. INTRODUCTION

An understanding of the dynamical behavior of liquid crystal directors including defects and transitions between topologically inequivalent states has become important for advanced liquid crystal modes, which can exhibit excellent electro-optical characteristics, such as an in-plane switch cell, patterned vertically aligned cell, multi-domain cell and so on. In order to understand defect dynamics, generally, two and three dimensional calculations that can include disclination for liquid crystal cells are important.

Previous papers [1,2] introduced the fast Q-tensor method which can handle defect dynamics in addition to normal liquid crystal behavior and topological transition. Dickman had shown that Oseen-Frank vector representation could go directly to the Q-tensor representation if we use only one 3rd order Q component [3]. However, Dickman considered only a constant value of order parameter S, so that the results are only qualitative in their description of defects. We have successfully shown that the fast Q-tensor method calculates the order parameter by adding the temperature terms in addition to the Q-tensor representation of Oseen-Frank free energy terms [1]. Besides, we have derived an improved normalization method for the faster calculations.

Defects in the LC director field sometimes occur due to surface inhomogeneity in addition to topologically inequivalent transition, because it can derive high elastic

energy around at "high changed position." Fig. 1 is a cartoon that shows the defect nucleation and defect lines at a prominence of the surface in the homeotropic aligned liquid crystal director field [4].

In this paper, we model the defect from surface prominence shown in Fig. 1 using fast Q-tensor representation. In order to confirm the calculated result, we compared the numerical modeling of the defect nucleation with experimental phenomenon. In addition, dynamical behaviors of the defect from surface inhomogeneity have been calculated under applied voltages.

## II. NUMERICAL MODELING OF A FAST Q TENSOR METHOD

The Gibb's free energy density ( $f_g$ ) consists of the ela-

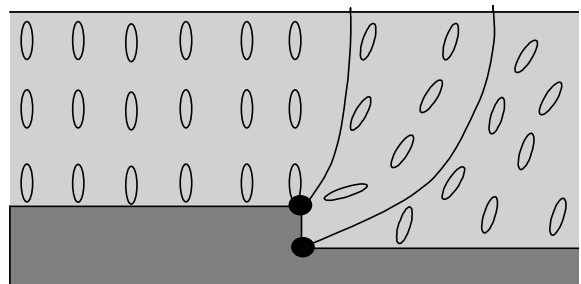


FIG. 1. Example of the decoration of mechanical inhomogeneities at a prominence by a nematic liquid crystal.

stic energy density term of the LC director ( $f_s$ ) and the external electric free energy density term ( $f_e$ ). Simply, we can achieve the total energy by integrating the calculated Gibb's free energy density. As I mentioned above, Dickman successfully derived the Q-tensor form from the vector form of the Frank-Oseen strain free energy density as below [5],

$$f_s = \frac{1}{12}(k_{33} - k_{11} + 3k_{22}) \frac{G_1^{(2)}}{S^2} + \frac{1}{2}(k_{11} - k_{22} - 3k_{24}) \frac{G_3^{(2)}}{S^2} + \frac{1}{2}k_{24} \frac{G_4^{(2)}}{S^2} + \frac{1}{6}(k_{33} - k_{11}) \frac{G_6^{(3)}}{S^3} + q_0 k_{22} \frac{G_4^{(2)}}{S^2} \quad (1)$$

$$G_1^{(2)} = Q_{jk,l} Q_{jk,l}, \quad G_2^{(2)} = Q_{jk,k} Q_{jl,l}$$

$$G_3^{(2)} = Q_{jk,l} Q_{jl,k}, \quad G_4^{(2)} = e_{jkl} Q_{jm} Q_{jm,l}$$

$$G_6^{(3)} = Q_{jk} Q_{lm,j} Q_{jm,k}$$

where  $Q_{jk} = S(n_j n_k - \frac{\delta_{jk}}{3})$ ,  $Q_{jk,l} = \frac{\partial Q_{jk}}{\partial l}$

The electric free energy density for the Q-tensor form is derived directly from  $f_e = D \cdot E/2$ . From this, the Q-tensor form for the electric free energy density can be obtained as below [5],

$$f_e = \frac{1}{2} \epsilon_0 (\bar{\epsilon} V_j^2 + \Delta \epsilon V_j V_{j,k} \frac{Q_{jk}}{S}) = \frac{2\epsilon_{\perp} + \epsilon_C}{3},$$

$$\Delta \epsilon = \epsilon_{\perp} - \epsilon_C, \quad V_j = \frac{\partial V}{\partial j} \quad (2)$$

In order to calculate the order parameter S in each grid, we need to add a temperature energy term that, in the absence of director field distortion, determines S as a function of temperature because the order parameter S is related directly to temperature. Basically, we can formulate the thermal energy density by using a simple polynomial expansion which is expressed as follows [6],

$$f_1(T) = f_0 + \frac{1}{2} A(T) Q_{ij} Q_{ji} + \frac{1}{3} B(T) Q_{ij} Q_{jk} Q_{ki} + \frac{1}{4} C(T) (Q_{ij} Q_{ij})^2 + O(Q^5) \quad (3)$$

Therefore, the total free energy density is the sum of equations (1), (2) and (3), so that the Gibb's free energy density can be described as the sum of these three energy densities.

In order to achieve the equilibrium state of the director configuration at constant electric field, it is typical to use the Euler-Lagrange equation. The following equations show the Euler-Lagrange representation for the electric potential and the director components under the Cartesian coordinate system. By solving eq. (4), potential distribution and LC configurations can be obtained.

$$0 = -[f_g]_{Q_{jk}}$$

$$0 = -[f_g]_V = \nabla \cdot D$$

where

$$[f_g]_{Q_{jk}} = \frac{\partial f_g}{\partial Q_{jk}} - \frac{d}{dx} \left( \frac{\partial f_g}{\partial Q_{jk,x}} \right) - \frac{d}{dy} \left( \frac{\partial f_g}{\partial Q_{jk,y}} \right) - \frac{d}{dz} \left( \frac{\partial f_g}{\partial Q_{jk,z}} \right)$$

$$[f_g]_V = \frac{\partial f_g}{\partial V} - \frac{d}{dx} \left( \frac{\partial f_g}{\partial V_x} \right) - \frac{d}{dy} \left( \frac{\partial f_g}{\partial V_y} \right) - \frac{d}{dz} \left( \frac{\partial f_g}{\partial V_z} \right) \quad (4)$$

The terms  $[f_g]_{Q_{jk}}$  and  $[f_g]_V$  represent the functional derivatives with respect to the  $Q_{jk}$  and voltage  $V$ , respectively. By using these equations, we can calculate the components of the 3 by 3 Q matrix and the voltages in each grid. Functional derivatives by each energy term are described as follows [2],

$$[f_g]_{Q_{jk}} = \text{strain term}([f_g]_S) + \text{voltage term}([f_g]_V) + \text{temperature term}([f_g]_T) \quad (5)$$

$$[f_g]_S = -\frac{2}{S^2} \left( -\frac{1}{12} K_{11} + \frac{1}{4} K_{22} + \frac{1}{12} K_{33} \right) Q_{jk,ll} + \frac{(K_{11} - K_{22})}{S^2} Q_{j,lk} - \frac{K_{24}}{S^2} Q_{j,lk} + \frac{1}{4S^3} (K_{33} - K_{11}) (Q_{lm,j} Q_{lm,k} - Q_{lm,l} Q_{jk,m} - Q_{lm} Q_{jk,ml} - Q_{lm,m} Q_{jk,l} - Q_{lm} Q_{jk,lm}) + \frac{2}{S^2} q_0 K_{22} j_{lm} Q_{mk,l}$$

$$[f_g]_V = -\frac{1}{2} \epsilon_0 D_e V_j V_{j,k}$$

$$[f_g]_T = (A_1 + A_2 \frac{T}{T_{ni}}) Q \cdot Q + A_3 Q \cdot Q \cdot Q + A_4 Q \cdot Q \cdot Q \cdot Q$$

$$Q_{jk,ll} = \frac{\partial}{\partial l} \left( \frac{\partial Q_{jk}}{\partial l} \right)$$

Where,  $T$  is the current temperature,  $T_{nj}$  represents the nematic-isotropic transition temperature, and the constants from  $A_1$  to  $A_4$  represent the coefficients for the polynomial equation. Generally, polynomial coefficients may be dependent on nematic material. The polynomial coefficients  $A_1$  to  $A_4$  have been adjusted so the  $T_{ni}$  are around 95 °C, so that we can see order parameter  $S$  and all diagonalized Q components go to 0 at  $T_{ni}$  from the typical value of room temperature (25 °C). As a result, we calculated that the polynomial coefficients  $A_1$ ,  $A_2$ ,  $A_3$  and  $A_4$  are 0.79 J/Cm<sup>3</sup>, 0.784 J/Cm<sup>3</sup>, 0.61 J/Cm<sup>3</sup> and 1.474 J/Cm<sup>3</sup>, respectively.

The dynamic equation  $\gamma(\partial Q_{jk}/\partial t) = -[f_g]_{Q_{jk}}$  can provide the equilibrium state by recalculating the Q-tensor and voltages in every time step in each grid.  $\gamma$  is rotational viscosity and we ignored bulk viscosity because have not considered flow effects. To obtain an equilibrium state, we applied a relaxation method based on dynamic equation for numerical calculation. As a result, the formulated relation between Q tensor of next time  $Q_{jk}^{-\tau+1}$  and that of current time  $Q_{jk}^{-\tau}$  is as follows,

$$Q_{jk}^{-\tau+1} = Q_{jk}^{-\tau} + \frac{\Delta t}{\gamma} [f_g]_{Q_{jk}} \quad (6)$$

The order parameter  $S$  is related to Q-tensor in the equation by  $S^2 = 2(Q \times Q)/3$  and we can get this simultaneously with the Q components.

### III. NUMERICAL MODELING FOR THE DEFECT NUCLEATION AND DYNAMICAL BEHAVIORS

De Gennes and Prost mentioned that the size of the defect core might approach molecular dimensions [6], so that we may encounter a serious problem for observing the defect core in the LC configuration. In the previous papers [1,2] we proposed a numerical method to find the defect core out by reducing the temperature coefficients  $A_1$  to  $A_4$ . In order to achieve the value of the coefficients, we can try to fit  $S$  as a function of temperature  $T$  to experimental data. Here, the coefficients are adjusted so  $T_{ni}$  is at 95 °C, and so  $S$  as to be 0.6 at room temperature. Specifically, the value of  $A_1$ ,  $A_2$ ,  $A_3$  and  $A_4$  as 0.79 J/Cm<sup>3</sup>, 0.784 J/Cm<sup>3</sup>, 0.61 J/Cm<sup>3</sup> and 1.474 J/Cm<sup>3</sup>, respectively, were determined. Otherwise, we need to scale down the cell structure for calculation. These two approaches obviously allow us to observe defect generation and dynamic behavior. Fig. 2 shows precise temperature characteristics of an order parameter  $S$  when we apply a voltage to the cell. It can be seen that by adjusting the coefficients  $A_1$  to  $A_4$  that give the ratio of the coefficients of the temperature terms to the other terms in the free energy equation, that the effect of a voltage on the phase transition temperature can be adjusted to meet an experimental result.

Fig. 3 (a) shows the geometry of the vertical aligned

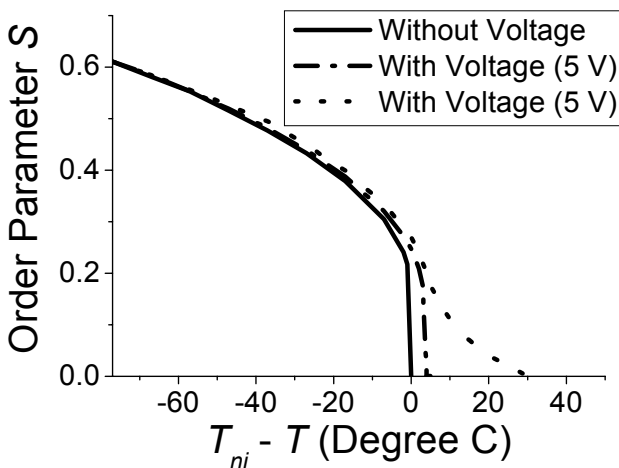


FIG. 2. The calculated dependence of the order parameter  $S$  on temperature  $T$ . The solid line represents results when no voltage is applied, the dash-dotted line and the dotted line represents the calculated results when we apply the 5 V. For the dotted lines, the values of  $A_1$ - $A_4$  have been changed to 0.01 times the values.

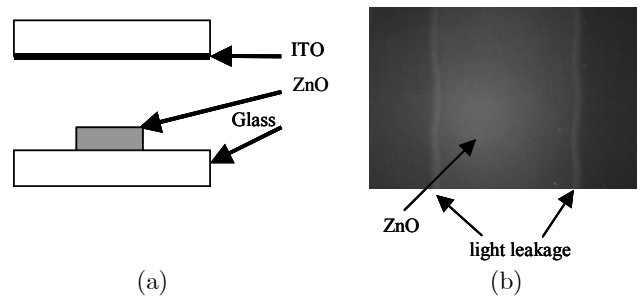


FIG. 3. An experiment for observing defect nucleation; (a) cell structure, (b) light leakage under crossed polarizers.

cell to realize the cell structure as shown in Fig. 1. The liquid crystal material was MLC-6608 of Merck Company ( $K_{11} = 16.7$  pN,  $K_{22} = 7.3$  pN,  $K_{33} = 18.1$  pN,  $\epsilon_{||} = 3.6$   $\epsilon_{\perp} = 7.8$ ). Cell gap to keep LC layer was 5  $\mu$ m, and ZnO layer was used for step surface configuration in a z-direction. Height of the ZnO layer was 1 $\mu$ m. Fig. 3 (b) shows microscopic photograph of the cell with crossed polarizers. From the figure, we have observed the light leakage from the edge of the electrode which implies nucleation of the defect core due to surface inhomogeneity with step type of the edge.

Fig. 4 (a) shows the cell geometry for simulating the defect nucleation from surface inhomogeneity. For the calculation, the number of calculated layers was set to

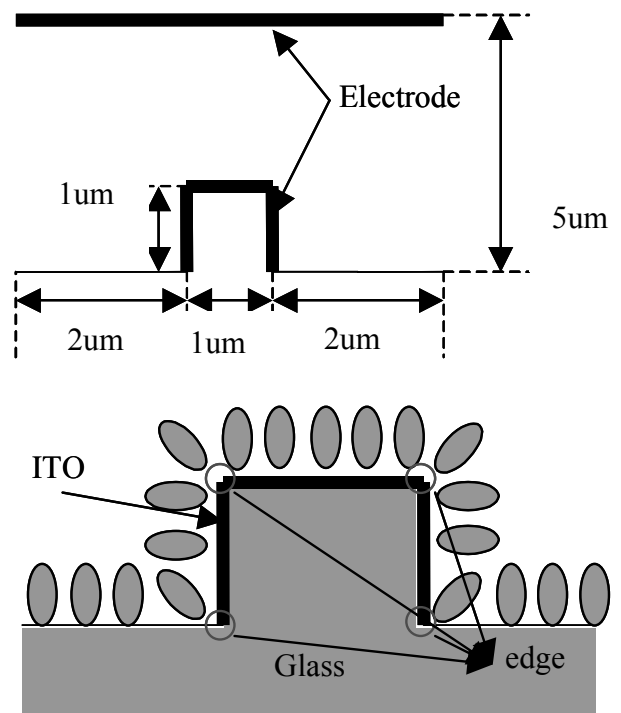


FIG. 4. The geometry of a vertical alignment LC cell for calculation; (a) cell structure, (b) LC alignment on the inhomogeneous surface.

$50 \times 50$  in the  $x$  and  $z$  directions. LC directors on the surface have aligned vertically and we assumed that the LC directors at corner grids of the edge have average numerical values of the neighbor directors as shown in Fig. 4 (b).

Fig. 5 shows the calculated result using the fast Q-tensor method. In the figure, length of the lines is proportional to amplitude of  $S$ , so that circled areas in the figure imply the points of defect nucleation. Without applied voltage as shown in Fig. 5 (a), defect was nucleated along the  $z$ -axis at the step side. This implies that high strain energy may be stored along the  $z$ -axis at the step side because the LC directors along the surface in the  $z$ -axis meet the LC directors in the bulk area with perpendicular state in a very short range. Fig. 5 (b), (c) and (d) show the dynamical behavior of the generated defects from surface inhomogeneity. It moves to the bulk area along defect line by applying the electric field. However, moving distance of the defects may be very short (under several  $\mu\text{m}$ ), so that we assume that the generated defects due to step surface inhomogeneity look stuck around the edge of the electrode even if we apply an electric field.

#### IV. CONCLUSIONS

Numerical modeling of the liquid crystal defect from surface inhomogeneity has been presented by using fast Q-tensor method. We modeled the defect nucleation near a prominence of the surface in the homeotropic liquid crystal director field. We confirm that defects can be generated due to surface inhomogeneity in addi-

tion to topologically inequivalent transition. For better optical characteristics of the LC cell, various structures of the LC cell may be applied to LC optical design and this may cause the unpredictable optical loss because of generated defects. A Fast Q-tensor method which provides information of the order parameter  $S$  may help us to understand defect dynamics and to design LC cells better.

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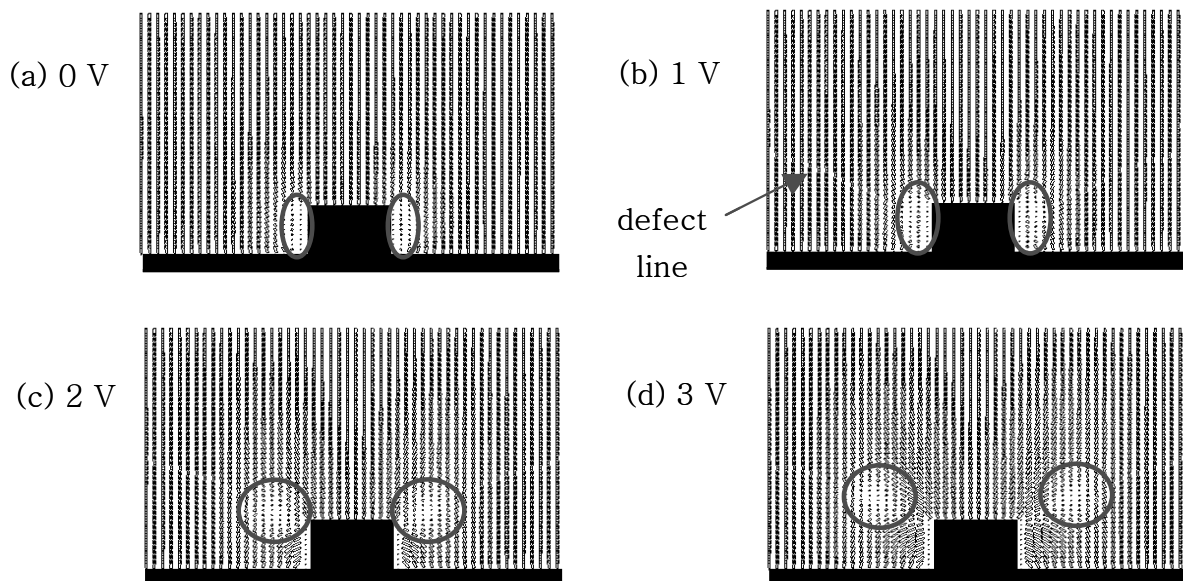


FIG. 5. Two-dimensional director configuration for a vertical alignment cell which includes inhomogeneous surface. The orientations of the cylinders give the local director orientation, which has very small order parameter  $S$ .

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