Numerical modeling of defects nucleation in the liquid crystal devices with inhomogeneous surface

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ABSTRACT

We model the nucleation and motion of defects in the liquid crystal display device with inhomogeneous surface by using fast Q-tensor method, which can calculate scalar order parameter S and nucleation of the defect in the liquid crystal director field. In order to model the defect, homeotropic aligned liquid crystal cell with step inhomogeneous electrode which has a height of 1 \( \mu \)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.

キーワード
liquid crystal, defect, surface inhomogeneity

I. Introduction

An understanding of the dynamical behavior of liquid crystal director 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 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 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 calculate 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 are occurred 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 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 calculated under applied voltages.

II. Numerical Modeling of a Fast Q tensor method

The Gibb's free energy density ($f_E$) consists of elastic energy density term of LC director ($f_E$) and external electric free energy density term ($f_0$). 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],

$$
\begin{align*}
\frac{e_0}{2} (K_{33}-K_{11}+3K_{22}) \frac{G_0^{(2)}}{S^2} & + \\
\frac{1}{2} (K_{11}-K_{22}-3K_{33}) \frac{G_0^{(2)}}{S^2} & + \frac{1}{2} K_{22} \frac{G_0^{(2)}}{S^2} \\
\frac{1}{6} (K_{33}-K_{11}) \frac{G_0^{(3)}}{S^2} & + \frac{1}{6} K_{22} \frac{G_0^{(3)}}{S^2}
\end{align*}
$$

(1)

$$
G_0^{(2)} = Q_{\mu\nu} Q_{\mu\nu}, \quad G_0^{(2)} = Q_{\mu\nu} Q_{\mu\nu} \quad G_0^{(3)} = Q_{\mu\nu} Q_{\mu\nu} Q_{\mu\nu} \\
G_0^{(3)} = Q_{\mu\nu} Q_{\mu\nu} Q_{\mu\nu} \quad G_0^{(3)} = Q_{\mu\nu} Q_{\mu\nu} \quad G_0^{(3)} = Q_{\mu\nu} Q_{\mu\nu} \quad G_0^{(3)} = Q_{\mu\nu} Q_{\mu\nu}
$$

where $Q_{\mu\nu} = S(n_{\mu} n_{\nu} - \frac{3}{r}), Q_{\mu\nu} = \frac{\partial Q_{\mu\nu}}{\partial r}$

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],

$$
\begin{align*}
\frac{f_E}{2} & = \frac{1}{2} \varepsilon_0 \varepsilon_{ij} V_{i,j}^2 + \Delta \varepsilon \varepsilon_{ij} V_{i,j} \frac{Q_{\mu\nu}}{S} \\
& = \frac{2 \varepsilon_{ij} + \varepsilon_C}{3}, \quad \Delta \varepsilon = \varepsilon_{ij} - \varepsilon_C, \quad V_{i,j} = \frac{\partial V}{\partial t}
\end{align*}
$$

(2)

In order to calculate order parameter $S$ in each grid, we need to add a temperature energy term that, in the absence of director field distortion, determine $S$ 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],

![Fig. 1. Example of the decoration of mechanical inhomogeneities at a prominence by a nematic liquid crystal](image-url)
\[ f_1 (T) = f_0 + \frac{1}{2} A(T) Q_{ij} Q_{ij} + \frac{1}{3} B(T) Q_{ij} Q_{jk} Q_{kl} \]
\[ + \frac{1}{4} C(T) (Q_{ij} Q_{ij})^2 + O(Q^3) \]  

(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, respectively.

\[ 0 = - \left[ f_x \right] \psi_x \]
\[ 0 = - \left[ f_x \right] \psi_v = \nabla \cdot D \]  

(4)

where

\[ \left[ f_x \right] \psi_x = \frac{\partial f_x}{\partial Q_{xx}} \cdot \frac{d}{dx} \left( \frac{\partial f_x}{\partial Q_{xx}} \right) + \frac{d}{dx} \left( \frac{\partial f_x}{\partial Q_{yy}} \right) - \frac{d}{dx} \left( \frac{\partial f_x}{\partial Q_{zz}} \right) \]

\[ \left[ f_x \right] \psi_v = \frac{\partial f_x}{\partial V_{xx}} \cdot \frac{d}{dx} \left( \frac{\partial f_x}{\partial V_{xx}} \right) + \frac{d}{dx} \left( \frac{\partial f_x}{\partial V_{yy}} \right) - \frac{d}{dx} \left( \frac{\partial f_x}{\partial V_{zz}} \right) \]

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

\[ [f_x]_{Qx} = \text{strain term}([f_x]_{Qx}) + \text{voltage term}([f_x]_{Vx}) + \text{temperature term}([f_x]_{Th}) \]

\[ [f_x]_{Qx} = \frac{2}{S^2} \left( \frac{1}{12} K_{xx} + \frac{1}{12} K_{xx} \right) \frac{Q_{xx}}{S} \]

\[ + \left( \frac{K_{xx} - K_{xx}}{S} \right) Q_{xx} - \frac{K_{xx} \cdot Q_{xx} - K_{xx} \cdot Q_{xx}}{S} \]

\[ + \left( \frac{K_{xx} - K_{xx}}{S} \right) Q_{xx} - \frac{Q_{xx} - Q_{xx}}{S} \]

\[ + \frac{2}{S} (K_{xx} - K_{xx}) Q_{xx} \]

\[ [f_x]_{Vx} = - \frac{1}{2} e D V_x \]

\[ [f_x]_{Vx} = (A + A \frac{T}{T_{th}}) Q_{xx} + A Q_{xx} Q_{xx} + A Q_{xx} Q_{xx} \]

Where, \(T\) is current temperature, \(T_a\) 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 that the \(T_a\) as to be around 95°C, so that we can see order parameter \(S\) and all diagonal \(Q\) components go to 0 at \(T_a\) from 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/cm3, 0.784 J/cm3, 0.61 J/cm3 and 1.474 J/cm3, respectively.

The dynamic equation \(\dot{Q}(\delta Q)\) can provide the equilibrium state by recalculation of the Q-tensor and voltages in every time step in each grid. \(\dot{r}\) is rotational viscosity. To obtain an equilibrium state, we applied relaxation method based on dynamic equation for numerical calculation. As a result, the formulated relation between Q tensor of next time \(Q_{jk}^{r+1}\) and that of current time \(Q_{jk}^{r}\) is as follows,

\[ Q_{jk}^{r+1} = Q_{jk}^{r} + \frac{\Delta t}{\gamma} [f_x] Q_{jk} \]  

(6)

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

III. Numerical modeling for the defect nucleation and dynamical behavior

De Gennes and Prost mentioned that the size of the defect core might be approached to 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 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 \( T_n \) is at 95 \(^\circ\)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\(^3\), 0.784 J/Cm\(^3\), 0.61 J/Cm\(^3\) and 1.474 J/Cm\(^3\), 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. Figure 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 coefficient \( A_1 \) 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.

![Diagram of a cell structure showing ITO and ZnO layers.](image)

**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.

Figure 3 (a) shows the geometry of the vertical aligned cell to realize the cell structure as shown in Fig. 1. Used liquid crystal material was MLC-6608 of Merck company (K11 = 16.77 pN, K22 = 7.33 pN, K33 = 18.1 pN, \( \epsilon \parallel = 3.6, \epsilon \perp = 7.8 \)). 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. Figure 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.

![Diagram of a vertical alignment LC cell structure showing electrodes and light leakage.](image)

**Fig. 3.** An experiment for observing defect nucleation: (a) cell structure, (b) light leakage under crossed polarizer

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which implies nucleation of the defect core due to surface
inhomogeneity with step type of the edge.

Figure 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
50×50 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).

Figure 5 shows calculated result using 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
z-axis at step side. This implies that high strain energy
may be stored along z-axis at step side because the LC
directors along surface in the z-axis meet LC directors in
bulk area with perpendicular state in a very short range.
Figure 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 μm), 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 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 by prominence of the surface in the homeotropic
liquid crystal director field. We confirm that defects can
be generated due to surface inhomogeneity in addition to
topologically inequivalent transition. For better optical
characteristics of the LC cell, various structure 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 cell better.

Reference

Q-tensor method for modeling liquid crystal director
configurations with defects", Appli.Phys. Lett. vol.81,
no. 21 pp.3951-3953, 2002.


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