액정 디스플레이 소자 내에서의 불균일한 표면에 의한 결점의 발생과 모델링

이기동* · 강봉순**

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

Gi-dong Lee* · Bongsoon Kang*

이 논문은 2005년도 동아대학교 교내학술연구비(공모과제)에 의해 연구되었음

요 약

액정 디스플레이 소자의 디렉터 내에서 결점을 모델링 할 수 있는 fast Q-텐서법을 이용하여 불균일한 표면에서 발생할 수 있는 결점의 발생과 움직임에 대한 모델링을 하였다. 결점을 모델링하기 위하여 1 μm 단차의 전극을 가진 수직배향셀을 이용하였다. 모델링을 통하여 단차에서 발생하는 액정 디렉터 내에서의 결점의 발생과 결점선을 확인할 수 있었으며 이러한 결과는 실험을 통하여 확인 하였다.

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 μm 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.

키워드

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

* 동아대학교 전자컴퓨터공학부 전임강사
** 동아대학교 전자컴퓨터공학부 부교수

접수일자 : 2005. 6. 21

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.

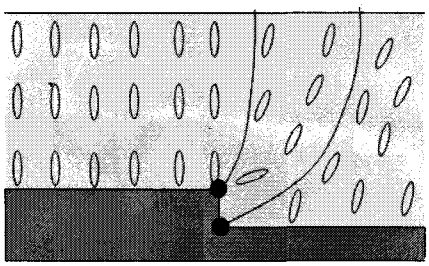


Fig. 1. Example of the decoration of mechanical inhomogenerities at a prominence by a nematic liquid crystal

Ⅱ. Numerical Modeling of a Fast Q tensor method

The Gibb's free energy density (f_g) consists of elastic energy density term of LC director (f_s) and 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],

$$
\begin{aligned}
fs = & \frac{1}{12}(K_{33}-K_{11}+3K_{22})\frac{G_1^{(2)}}{S^2}+ \\
& \frac{1}{2}(K_{11}-K_{22}-3K_{24})\frac{G_2^{(2)}}{S^2}+\frac{1}{2}K_{24}\frac{G_3^{(2)}}{S^2} \\
& +\frac{1}{6}(K_{33}-K_{11})\frac{G_6^{(3)}}{S^3}+q_0K_{22}\frac{G_4^{(2)}}{S^2} \qquad (1)
\end{aligned}
$$

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

$$
G_3^{(2)}=Q_{jk,l}\,Q_{jl,k},\ G_4^{(2)}=e_{jkl}Q_{jm}\,Q_{jm,l},\ G_6^{(3)}=Q_{jk}\,Q_{lm,j}Q_{lm,k}
$$

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

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

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

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],

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

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, respectively.

$$0 = -[f_g]_{Q_{jk}}$$
$$0 = -[f_g]_V = \nabla \cdot D \quad (4)$$

where

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

The terms $[f_g]_{Qjk}$ 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 voltages in each grid. Functional derivatives by each energy term are described as follows [2],

$[f_g]_{Qjk}$ = strain term($[f_g]_S$) + voltage term($[f_g]_V$) + temperature term($[f_g]_T$)

$$[f_g]_S = \frac{2}{S^2}\left(\frac{1}{12}K_{11} + \frac{1}{4}K_{22} + \frac{1}{12}K_{33}\right)Q_{jk,ll} + \frac{(K_{11}-K_{22})}{S^2}Q_{jl,lk} - \frac{K_{24}}{S^2}Q_{jl,lk} + \frac{1}{4S^3}(K_{33}-K_{11})(Q_{mj}Q_{mk,ll} - Q_{mj}Q_{lk,lm} - Q_{lm}Q_{jk,ml} - Q_{mm}Q_{jk,ll} - Q_{lm}Q_{jk,lm}) + \frac{2}{S^2}q_0K_{22}e_{jlm}Q_{mk,l}$$
$$[f_g]_V = -\frac{1}{2}e_0D_{e,j}V_{,k} \quad (5)$$
$$[f_g]_T = \left(A_1 + A_2\frac{T}{T_{ni}}\right)Q_{jk}Q_{kj} + A_3Q_{jk}Q_{kl}Q_{lj} + A_4Q_{jk}Q_{kl}Q_{lm}Q_{mj}$$
$$Q_{jk,ll} = \frac{\partial}{\partial l}\left(\frac{\partial Q_{jk}}{\partial l}\right)$$

Where, T is current temperature, T_{ni} 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} as to be around 95 °C, so that we can see order parameter S and all diagonalzed Q components go to 0 at T_{ni} 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 $\gamma(\partial Q_{jk}/\partial t) = -[f_g]_{Qjk}$ can provide the equilibrium state by recalculating the Q-tensor and voltages in every time step in each grid. γ 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 $Q_{jk}^{-\tau+1}$ and that of current time $Q_{jk}^{-\tau}$ is as follows,

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

The order parameter S is related to Q-tensor in the equation by $S^2 = 2(Q\cdot Q)/3$ 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_{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^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.

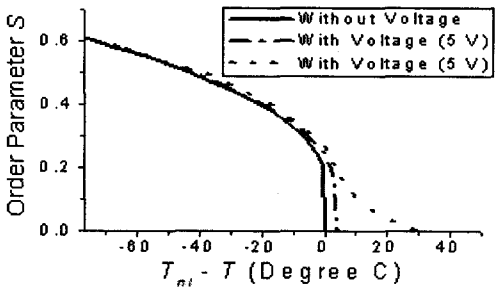
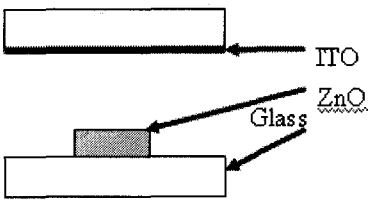
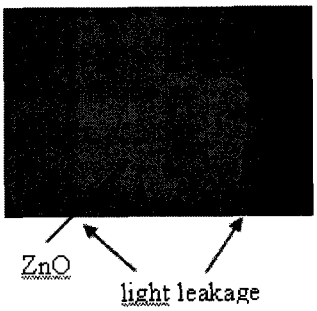


Fig. 2. The calculated dependence of the order parameter S on temperature T. The solid line represents results when no voltage is applied, the dash-dotted line and the dotted line represents the calculated results when we apply the 5 V. For the dotted lines, the values of A1-A4 have been changed to 0.01 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 = 16.7 pN, K22 = 7.3 pN, K33 = 18.1 pN, $\epsilon_{\parallel}$ = 3.6, $\epsilon_{\perp}$ = 7.8). Cell gap to keep LC layer was 5 μm, and ZnO layer was used for step surface configuration in a z-direction. Height of the ZnO layer was 1μm. 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

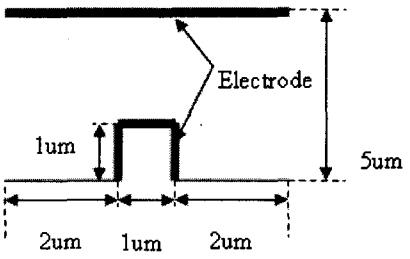


(a)

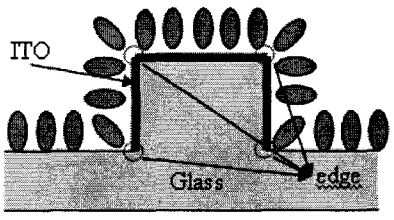


(b)

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



(a)



(b)

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

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.

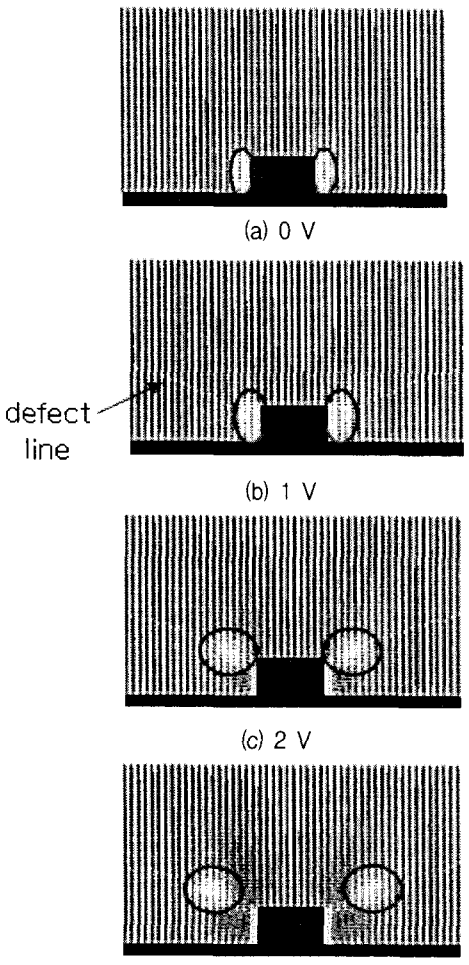


Fig.5. Two-dimensional director configuration for a vertical alignment cell which includes inhomogeneous surface. The orientations of the cylinders give the local director orientation, which has very small order parameter S.

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

[1] Gi-Dong Lee, James Anderson, Philip J. Bos, *"Fast Q-tensor method for modeling liquid crystal director configurations with defects"*, Appli.Phys. Lett. vol.81, no. 21 pp.3951-3953, 2002.

[2] G. D. Lee, P. J. Bos, S. H. Ahn, and K. H. Kim,

"Fast Q-tensor method for modeling the dynamics of defects in a liquid crystal director field", Phys. Rev. E, vol.67, pp.41715-41721, 2003.

[3] S. Dickmann : Ph. D. Dissertation, University Karlsruhe, Karlsruhe, Germany, 1995

[4] A. A. Sonin, The Surface Physics of Liquid Crystals, (Gordon and Breach Publishers, Newyork, USA), pp. 111-112.

[5] H. Mori, E. C. Gartland, J. R. Kelly, and P. J. Bos, *"Multidimensional Director Modeling Using the Q Tensor Representation in a Liquid Crystal Cell and Its Application to the pi Cell with Patterned Electrodes"*, Jpn. J. Appl. Phys. Vol. 38, no. 1A, pp.135-146, 1999.

[6] P. G. de Gennes and J. Prost, The Physicsof Liquid Crystals (Clarendon Press, Newyork, USA, 1993), pp. 165-185.

Authors

Gi-Dong Lee

1989 Bachelor degree in Dept. of Electronics Eng., Pusan National Univ.

1991 Master degree in Dept. of Electronics Eng., Pusan National Univ.

1991~1997 LCD R&D center in Samsung SDI

2000 Ph. D. in Dept. of Electronics Eng., Pusan National Univ.

2001~2003 Research Fellow, Liquid Crystal Institute in Kent State Univ.

2004~current Full-time instructor, School of Electronics and Computer Eng. in Dong-A University.

※ Interesting area : Display Devices

Bongsoon Kang

1985 Bachelor degree in Dept. of Electronics Eng., Yonsei Univ.

1987 Master degree in Dept. of Electrical Eng., University of Pennsylvania

1990 Ph.D. degree in Dept. of Electrical and Computer Eng., Drexel University

1989~1999 Senior Research Staff, R&D Center, System LSI Division, Samsung Electronics

1999~current Associate professor, School of Electronics and Computer Eng. in Dong-A University.

※Interesting area : System IC Design