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Simulation of the Optical Transmittance of IPS LC-Cell on Temperature Variation

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In this paper we calculated optical transmittance of the In-Plane Switching (IPS) liquid crystal (LC) cell with respect to temperature. By considering temperature energy term in the Gibb's free energy, we could achieve the temperature parameters that need to calculate the temperature dependence on the electro-optic characteristics. The calculated temperature parameters permit us to calculate scalar order parameter S with respect to temperature, so that finally we could calculate the optical transmittance of the IPS LC cell as a function of temperature.

Keywords: fast Q-tensor; IPS LC; liquid crystal; modeling; temperature

1. INTRODUCTION

Currently, liquid crystal (LC) cell has been widely used for applications such as display device and optical components. In order to predict and optimize the electro-optical characteristics of the LC cell before manufacturing, many approaches for modeling of the LC directors have been introduced and could provide the excellent calculation results. However, in terms of temperature properties of the LC cell, simulation methods introduced and commercialized before were scarcely able to calculate useful outputs because they could not

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calculate scalar order parameter S which is an only parameter of the temperature. In the previous papers [1,2], however, we have shown the fast Q-tensor method that can achieve the scalar order parameter S by adding the temperature energy term into the Dickman's tensor representation of the Oseen-Frank free energy terms [3]. The fast Q-tensor method considers the temperature energy term in addition to the elastic and electric energy term, so that it can provide the qualitative and quantitative modeling of the LC director field regarding defects, phase transition and even electro-optic characteristics on temperature because it can calculate the order parameter S in each position of the LC cell.

In this paper we calculated dependence of optical transmittance of the In-Plane Switching (IPS) liquid crystal (LC) cell [4] on temperature. In order to calculate the optical characteristics as a function of the temperature, we first calculate scalar order parameter S in each grid point of the cell. From the calculation, we could calculate the optical anisotropy of the cell in each temperature range. As a result, we could calculate the optical transmittance of the IPS LC cell as a function of temperature.

2. MODELING OF THE LC DIRECTOR USING THE FAST Q-TENSOR METHOD

Generally, 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). As I mentioned above, Dickman successfully directly derived the tensor representation from vector form of the Ossen-Frank free energy density in order to model the phase transition of the LC director between topologically inequivalent states as below [3,5].

$$f_s = \frac{1}{12}(K_{33} - K_{11} + 3K_{22})\frac{G_1^{(2)}}{S^2} + \frac{1}{2}(K_{11} - K_{22} - 3K_{24})\frac{G_2^{(2)}}{S^2} + \frac{1}{2}K_{24}\frac{G_3^{(2)}}{S^2} + \frac{1}{6}(K_{33} - K_{11})\frac{G_6^{(3)}}{S^3} + q_0 K_{22}\frac{G_4^{(2)}}{S^2} \tag{1}$$

$$f_e = \frac{1}{2}\varepsilon_0\left(\bar{\varepsilon}V_{,j}^2 + \Delta\varepsilon V_{,j}V_{,k}\frac{Q_{jk}}{S}\right)$$

$$\bar{\varepsilon} = \frac{2\varepsilon_\perp + \varepsilon_{\coprod}}{3}, \Delta\varepsilon = \varepsilon_\perp - \varepsilon_{\coprod}, V_{,j} = \frac{\partial V}{\partial j}$$

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

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

where

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

where K_{11}, K_{22}, and K_{33} represent the splay, twist and bend elastic constants, respectively. K_{24} is energy density related to surface anchoring energy. In the case of strong anchoring state, we can ignore the $K_{24.}$ The Levi-Civita symbol e_{ijk} is 1 when subscripts are in the order of *xyz, yzx*, or *zxy*, and is -1 if the subscript order is *xzy, yxz*, or *zyx*, 0 otherwise. The δ_{jk} is Kronecker's delta, which is 1 if j equals k, and 0 otherwise.

By using Eq. (1), we can model the phase transition between the topologically inequivalent states of the LC cell. However, Dickman's representation of the free energy density as shown in Eq. (1) considered only a constant value of order parameter S, so that the results are only qualitative in their description of defects.

In order to describe the quantitative result in addition to qualitative representation of the LC director, the fast Q-tensor method applied the temperature energy density term, which can be formulated by using a simple polynomial expansion in terms of the Q-tensor, to the Gibb's free energy density as below [6],

$$f_t(T) = f0 + \frac{1}{2}A(T)Q_{ij}Q_{ji} + \frac{1}{3}B(T)Q_{ij}Q_{jk}Q_{ki} + \frac{1}{4}C(T)(Q_{ij}Q_{ij})^2 + O(Q^5) \tag{2}$$

Therefore, the total free energy density is the sum of Eqs. (1) and (2), so that the Gibb's free energy density can be described as the sum of these three energy densities. In this equation, we can successfully calculate the scalar order parameter S as a variable in each grid of the LC cell by adding up the temperature energy density term. Therefore, once we get the scalar order parameter S in each grid position, we can simply calculate change of the optical anisotropy in each grid position on temperature either.

Generally, the equilibrium state of the director configuration is typically achieved by using the Euler-Lagrange equation. The Euler-Lagrange equation for the electric potential and the director components can be described as follows [3],

$$\begin{aligned} 0 &= -[f_g]_{Q_{jk}} \\ 0 &= -[f_g]_V = \nabla \cdot D \end{aligned} \tag{3}$$

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 9 components of Q matrix and voltages in each grid. The functional derivative equations for calculation of the Eq.(3) are described as follows [2],

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

$$[f_g]_S = -\frac{2}{s^2}\left(-\frac{1}{12}K_{11} + \frac{1}{4}K_{22} + \frac{1}{12}K_{33}\right)Q_{jk,ll} + \frac{(K_{11} - K_{22})}{S^2}Q_{jl,lk}$$
$$-\frac{K_{24}}{S^2}Q_{jl,lk} + \frac{1}{4S^3}(K_{33} - K_{11})(Q_{lm,j}Q_{lm,k} - Q_{lm,l}Q_{jk,m}$$
$$- Q_{lm}Q_{jk,ml} - Q_{lm,m}Q_{jk,l} - Q_{lm}Q_{jk,lm}) + \frac{2}{S^2}q_0K_{22}e_{jlm}Q_{mk,l} \quad (4)$$
$$[f_g]_T = \left(A_1 + A_2\frac{T}{T_{ni}}\right)Q \cdot Q + A_3 Q \cdot Q \cdot Q + A_4 Q \cdot Q \cdot Q \cdot Q$$
$$Q_{jk,ll} = \frac{\partial}{\partial l}\left(\frac{\partial Q_{jk}}{\partial l}\right)$$

here, T is temperature, T_{ni} represents the nematic-isotropic transition temperature, and the constants from A_1 to A_4 represent the coefficients for the curve fitting polynomial. Generally, polynomial coefficients may be dependent on material properties of the LC material. In order to achieve the value of the coefficients, we can try to fit S as a function of temperature T to experimental data. Therefore, once we know the value of the T_{ni} and the scalar order parameter at room temperature, we can calculate the temperature coefficients, so that we can fit the S curve as a function of the temperature.

3. SIMULATION OF THE OPTICAL TRANSMITTANCE OF THE IPS-LC CELL

In order to calculate the temperature dependence of the LC cell, we applied fast Q-tensor method to IPS LC cell. Used LC material for calculation is ML-0249, which has 75°C of T_{ni} and 0.104 of optical anisotropy Δn. We assume the scalar order parameter at room temperature (25°C) as 0.6. Therefore, the coefficients are adjusted so T_{ni} is at 75°C, and so S as to be 0.6 at room temperature. As a result, we could calculate the value of A_1, A_2, A_3, and A_4 as $A_1^0 = -0.784$ J/cm^3, $A_2^0 = 0.93$ J/cm^3, $A_3^0 = -0.7$ J/cm^3, and $A_4^0 = 1.0$ J/cm^3, respectively,

Figure 1 shows the precise temperature characteristics of an order parameter S 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. From the figure, we can observe that the effect of temperature on the phase transition can be adjusted to meet an experimental result.

In order to calculate the optical transmittance of the LC cell with respect to temperature, we need to describe the optical anisotropy in each grid position as a function of the scalar order parameter S. In general, the optical anisotropy can be represented as $\Delta n \propto S\rho^2$ [7]. Here, S is the scalar order parameter and ρ represents the material density.

Therefore, this equation indicates scalar order parameter and square-root of the density have linear relation with optical anisotropy. This relation does not always show adjutancy with experimental result. However, we assume the linearity of the optical anisotropy with the scalar order parameter in this calculation.

Therefore, the calculated optical anisotropy can be described as below,

$$\Delta n = \frac{S}{S_o} \times \Delta n_o \tag{5}$$

where, Δn_o and S_o represent optical anisotropy and the scalar order parameter at room temperature (25°C), respectively.

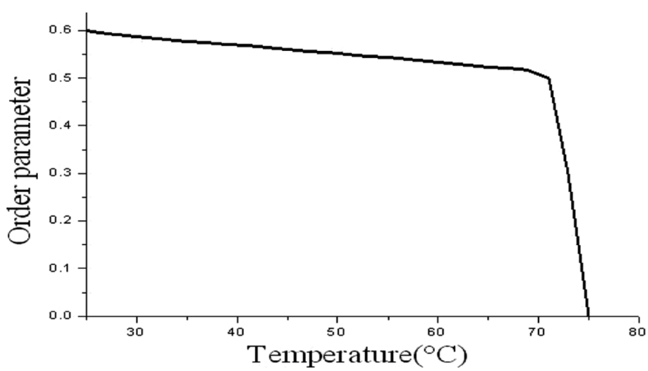

FIGURE 1 calculated scalar order parameter of the used LC ML-0249 as a function of temperature.

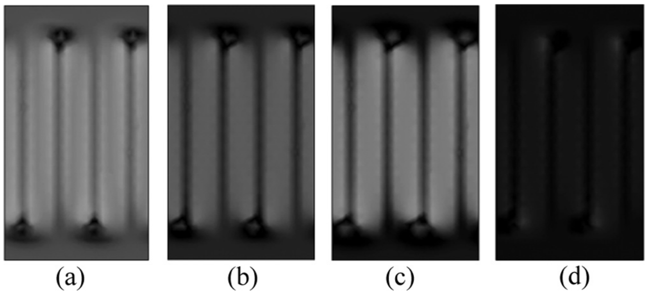

FIGURE 2 calculated optical intensity of the IPS LC cell as a function of temperature: (a) 0°C, (b) 25°C, (c) 45°C, (d) 75°C.

Optical transmittance of the IPS LC cell with respect to temperature can be simply achieved by the calculated output optical anisotropy from Eq. (5). Figure 2 shows the calculated optical intensity of the IPS LC cell in the bright state in each given temperature (0°C, 25°C, 45°C, and 75°C). The applied voltage to the IPS LC cell under crossed polarizer is 7 volt. Optical anisotropy in each temperature can be obtained by using the result of Figure 1 and Eq. (5). From the Figure 2, we can observe the decrease of the light intensity of the LC cell as the temperature become high because of the decrease of the scalar order parameter. However, we also observe that the light intensity does not get perfect dart state even if the temperature goes to nematic-isotropic point

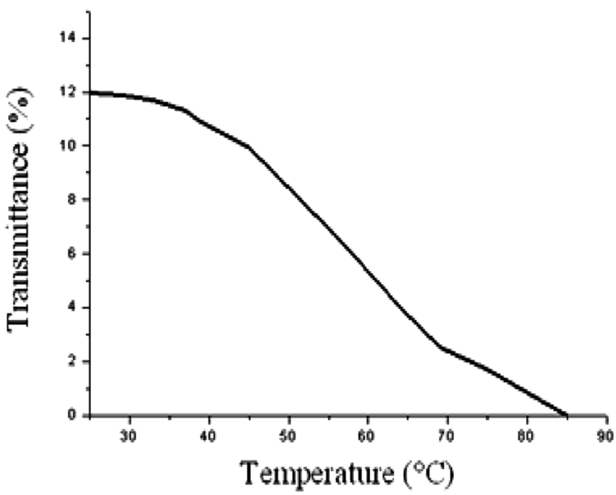

FIGURE 3 calculated optical transmittance of the IPS LC cell as a function of temperature.

because the LC director field does not become isotropic state due to the applied voltage, so that the scalar order parameter does not be zero even if temperature becomes nematic-isotropic position. Effect of the applied voltage on the scalar order parameter was observed in the previous paper [2].

Figure 3 shows the calculated optical transmittance of the IPS LC cell as a function of temperature. We observed that the transmittance of the cell becomes zero at 85°C because of the applied voltage.

4. CONCLUSION

In this paper we simulated optical characteristics of the IPS LC cell as a function of temperature. In order to calculate the optical transmittance of the LC cell, we first calculated scalar order parameter S as a variable in each grid position by using the fast Q-tensor method. By applying the linear relationship between the optical anisotropy and the scalar order parameter S, we simply calculated optical anisotropy in the given temperature. As a result, we could simulate the electro-optical characteristics from the calculated result on the optical anisotropy. The paper indicates that the dependence of electro-optic characteristics of the LC cell on the applied temperature can be easily obtained by calculating the scalar order parameter by using the fast Q-tensor method.

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