Q 텐서 기법을 이용한 원 형태의 액정 구조체 디렉터 분포

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Circular Liquid Crystal Director Field Using Q-tensor Method

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요 약

We calculate liquid crystal director field in circularly confined capsules by using Q-tensor method [2, 3], which can calculate not only the LC director field in bulk area but the local phase transition in high elastic distortion area. We calculated LC director filed in colloidal capsule with the boundary condition of both homogeneous state and homeotropic state in this paper.

I. 서 론

Liquid crystal displays (LCDs) have been widely used in various application such as mobile phones, personal computers (PCs), televisions (TVs) in flat panel display, because liquid crystal display (LCD) technology has been developed by studying in a variety of LC characteristics including viewing angle, response time, contrast ratio, etc. Nowadays, flexible panel display and flat panel display are really important in display industry. However, Liquid crystal displays (LCDs) are not possible to bend because it has a structure filled liquid crystal between two glass substrates. To solve this problem, nano-sized liquid crystal capsule is studied [1], extremely small size of LC droplets embedded in the nanoencapsulated layer, less than a quarter of wavelength of incident light, appear transparent in the voltage, exhibiting the optical behavior of uniaxial retarder. Because the non-existence of simulation tools we still don't know about the liquid crystal director in circularly confined capsules.

In this paper, we calculate liquid crystal director field in circularly confined capsules by using Q-tensor method [2], which can calculate not only the LC director field in bulk area but the local phase transition in high elastic distortion area. We calculated LC director filed in colloidal capsule with the boundary condition of both homogeneous state and homeotropic state [3].

II. 본 론

The Gibb"s free energy density (fg) consists of elastic energy density term of LC director (fs) and external electric free energy density term (fe). 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 :

$$\begin{aligned} f_s &= \frac{1}{12}(K_{33}-D_{11}+3K_{22})\frac{G_1^{(2)}}{S^2} \\ &\quad +\frac{1}{2}(K_{11}-K_{22}-3K_{24})\frac{G_2^{(2)}}{S^2}+\frac{1}{2}K_{24}\frac{G_3^{(2)}}{S^2} \\ &\quad +\frac{1}{6}(K_{33}-K_{11})\frac{G_6^{(2)}}{S^3}+q_0K_{22}\frac{G_4^{(2)}}{S^2}, \\ G_1^{(2)} &= Q_{jk,l}Q_{jk,l}, \quad G_2^{(2)}=Q_{jk,k}Q_{jl,l}, \\ G_3^{(2)} &= Q_{jk,l}Q_{jl,k}, \quad G_4^{(2)}=e_{jkl}Q_{jm}Q_{jm,l}, \\ G_6^{(2)} &= Q_{jk}Q_{lm,j}Q_{lm,k}, \\ Q_{jk} &= S\left(n_jn_k-\frac{\delta_{jk}}{3}\right), \quad Q_{jk,l}=\frac{\partial Q_{jk}}{\partial l}, \end{aligned} \tag{1}$$

where K11, K22, and K33 are the splay, twist and bend constants, respectively. K24 is associated with the surface anchoring energy. If we assume that the LC directors are fixed at the surface layer, K24 can be ignored. The q0 is the LC chirality. The Levi-Civita symbol eijk is 1 when subscripts are in the order of xyz, yzx, or zxy, is −1 when the subscript order is xzy, yxz, or zyx, and is 0 otherwise. The δjk is the Kronecker delta, which is 1 if j equals k, and is 0 otherwise.

The electric free energy density for the Q-tensor form is derived directly from fe = D·E/2. From this, the Q-tensor form for the electric free energy density can be obtained as below :

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

Therefore, the total free energy density is the sum of equations (1) and (2), so that the Gibb"s free energy density can be described as the sum of these two 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 which is 0 = −[fg]Qjk and 0 = −[fg]V = ▽·D. The terms [fg]Qjk and [fg]V represent the functional derivatives with respect to the Qjk 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 :

$$\begin{aligned} [f_g]_{Q_{jk}} &= \text{strain term}([f_g]_S)+\text{voltage term}([f_g]_V) \\ [f_g]_S &= -2\left(-\frac{1}{12}K_{11}+\frac{1}{4}K_{22}+\frac{1}{12}K_{33}\right)Q_{jk,ll} \\ &\quad -(K_{11}-K_{22}-K_{33})Q_{jl,lk}-K_{24}Q_{jl,lk} \\ &\quad +\frac{1}{4}(K_{33}-K_{11})(Q_{lm,j}Q_{lm,k}-Q_{lm,l}Q_{jk,m} \\ &\quad -Q_{lm}Q_{jk,ml}-Q_{lm,m}Q_{jk,l}-Q_{lm}Q_{jk,lm}) \\ &\quad +2q_0K_{22}e_{jlm}Q_{mk,l}, \\ [f_g]_V &= -\frac{1}{2}e_0D_eV_{,j}V_{,k}, \\ Q_{jk,ll} &= \frac{\partial}{\partial l}\left(\frac{\partial Q_{jk}}{\partial l}\right), \end{aligned} \tag{3}$$

The tensor and voltages at each grid point should be recalculated in every time step until they exhibit stable response. We can achieve this by using the dynamic equation $\gamma(\partial Q_{jk}/\partial t)=-[f_G]_{Q_{jk}}$, where γ is rotational viscosity. And we ignored bulk viscosity because have not considered flow effect. The formulated relation between Q tensor of next time $Q_{jk}^{-\tau+1}$ and that of current time $Q_{jk}^{-\tau}$ is as follows:

$$Q_{jk}^{-\tau+1}=Q_{jk}^{-\tau}+\Delta t[f_g]Q_{jk}/\gamma \tag{4}$$

Using this equation, the Q-tensor components can be updated at each time step, so that the final static value of the Q-tensor is the equilibrium state.

III. 실험 및 결과

Figure 1 shows the results of simulation. The liquid crystal material used simulation is

ZLI-1565 with K11=14.4pN, K22=6.9pN, K33=18.3pN, $\varepsilon_{\parallel}$ =10.7, $\varepsilon_{\perp}$ =3.7. No chiral agent is added, which means q0 =0. The pretilt angle of bottom and top surface is 5° and −5°, respectively.

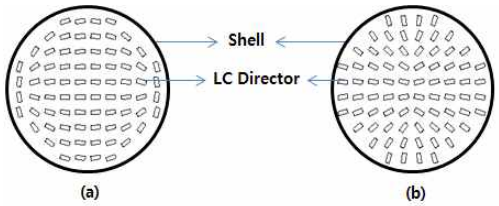

Figure 1. LC director filed in colloidal capsule with the boundary condition of both (a) homogeneous state and (b) homeotropic state

IV. 결 론

In conclusion, we have studied dynamical behavior of LC director field by using a Q-tensor method. It allows us to understand LC director filed in colloidal capsule with the boundary condition of both homogeneous state and homeotropic state. The calculated results explain well the experimental behavior.

감사의 글

This paper was supported by LG Display and Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (2015R1D1A3A03020569)

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