Chemical Physics Publications   Department of Chemical Physics

Fast Q-Tensor Method for Modeling the Dynamics of Defects in a Liquid Crystal Director Field

Philip J. Bos
Kent State University - Kent Campus, pbos@kent.edu

Gi-Dong Lee
Kent State University - Kent Campus

Seon Hong Ahn

Kyeong Hyeon Kim

Recommended Citation

Fast *Q*-tensor method for modeling liquid crystal director configurations with defects

Gi-Dong Lee, James Anderson, and Philip J. Bos[a)]

Liquid Crystal Institute, Kent State University Kent, Ohio 44242

A fast *Q*-tensor method, which can model the configuration of the liquid crystal director fields containing defects, is proposed. Conceptually based on the Oseen–Frank approach, we have added temperature energy density terms in addition to the strain energy term. We have also derived an improved normalization method for fast calculations. The method is used to model the conversion of a reverse tilt wall to a pair of disclination lines. © *2002 American Institute of Physics.*
[DOI: 10.1063/1.1523157]

An understanding of the dynamic behavior of liquid crystal (LC) director fields including defects and transitions between topologically inequivalent states has become important for the LC device modes such as the Pi-cell,[1] multidomain cell, patterned vertically aligned cell,[2] as well as conventional defect-free LC mode such as the twisted nematic cell. Defects or disclinations often result from nonuniform electric field distributions due to patterned electrodes. In other cases, the operation of a device may depend on the nucleation of a defect to allow for the transition between topologically inequivalent director configurations. So, two- and three-dimensional calculations that can include disclinations for liquid crystal cells are important for the understanding of these types of devices.

Generally, the Gibb's free energy of the LC cell is minimized in order to achieve the configuration of LC directors in the equilibrium state. It consists of elastic deformation terms and electric field terms. The elastic deformation energy can be expressed with Oseen–Frank vector representation, which use three elastic constants (splay, twist, and bend). The Oseen–Frank vector representation, however, cannot handle defects that may happen in the LC cell because it assumes that the order parameter S is a constant, and when discretized, it depends on the sign of the unit vector describing the director field.

An alternative method, the Landau–de Gennes's Q representation[3] can handle the defects and phase transitions in addition to the normal dynamic behavior of LC cells by combining the thermal and strain free energy. In the Q-tensor method, two elastic constants are yielded if we use the second order Q-tensor expansion. However, it has been proved that degeneracy between splay and bend elastic constants can be removed if we use the third order expansion, so that three elastic constants can be achieved.[4] Berreman has shown the relation between the Oseen–Frank elastic terms and second and third order terms and mentioned only one among the third order parameters is needed for removing the degeneracy.[5]

Also, Dickman has shown that Oseen–Frank vector representation could go directly to the Q-tensor representation if we use only one third order Q component.[6] However, Dickman considered only a constant value of order parameter S, and therefore cannot yield a quantitative description of a director configuration containing defects.

In this letter, Dickman's Q-tensor method is extended to develop a computational method of the liquid crystal director configuration that can handle defects, and that is clearly based on the three elastic constants of the Oseen–Frank free energy. For the calculation of the order parameter S, we added the temperature energy terms[3] in addition to the Q-tensor representation of Oseen–Frank free energy terms. We have also derived an improved normalization method for fast calculation.

As mentioned before, the Frank–Oseen strain free energy density can be changed to Q-tensor representation directly. The strain energy density fs is

$$
\begin{aligned}
fs = {} & \frac{1}{12}(k_{33}-k_{11}+3k_{22})\frac{G_1^{(2)}}{S^2} + \frac{1}{2}(k_{11}-k_{22} \\
& -3k_{24})\frac{G_2^{(2)}}{S^2} + \frac{1}{2}k_{24}\frac{G_3^{(2)}}{S^2} + \frac{1}{6}(k_{33}-k_{11})\frac{G_6^{(3)}}{S^3} \\
& + q_0 k_{22}\frac{G_4^{(2)}}{S^2},
\end{aligned}
$$

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

$$
G_3^{(2)} = Q_{jk,l}Q_{jl,k}, \quad G_4^{(2)} = e_{jkl}Q_{jm}Q_{jm,l}, \tag{1}
$$

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

where Q_{jk} are the components for the tensor order parameter that are defined by $S(n_j n_k - \delta_{jk}/3)$. 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. The Q tensor is not written in a vector notation and so does not give nonphysical energies around a $S=1/2$ disclination.[3,6] In spite of this merit, this method cannot model the dynamic LC configuration including defects because it has always a constant order parameter S that is equal to the value of S at the temperature where the elastic constants were measured.

In order to understand the dynamical behavior surrounding defects such as disclinations in a LC cell, we need to use the information on the order parameter S at the each grid

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[a)]Author to whom correspondence should be addressed; electronic mail: pbos@kent.edu

point. The order parameter S is related directly to temperature, and we need to add a temperature energy term that, in the absence of director field distortion, determine S as a function of temperature. Basically, we can formulate the thermal energy density by using a polynomial expansion in terms of the Q tensor that is expressed as follows:[3]

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

From Eqs. (1) and (2), we can recognize that the sum of these terms are analogous to de Gennes's Q tensor expression of thermal and strain free energy in the absence of electric field for uniaxial cholesterics. The restriction to a uniaxial order parameter tensor maybe considered inappropriate in regions where the order parameter is spatially varying. However, it is experimentally observed that the size of the region where the order parameter is spatially varying is typically on the order of molecular dimensions, and the importance of the distinction between uniaxiality or biaxiality over such a small region may not be expected to have a large effect on the outcomes of the problems considered here.

The electric free energy density f_e or the Q-tensor form is derived directly from $f_e = \mathbf{D} \cdot \mathbf{E}/2$. From this, the Q-tensor form for the electric free energy density can be obtained easily as shown later

$$f_e = \frac{1}{2}\epsilon_0\left(\bar{\epsilon}V_{,j}^2 + \Delta\epsilon V_{,j}V_{,k}\frac{Q_{jk}}{S}\right)$$
$$\bar{\epsilon} = \frac{2\epsilon_\perp + \epsilon_\parallel}{3}, \quad \Delta\epsilon = \epsilon_\perp - \epsilon_\parallel, \quad V_{,j} = \frac{\partial V}{\partial j}. \qquad (3)$$

The total free energy density is the sum of Eqs. (1), (2), and (3). 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 Euler–Lagrange equations for the electric potential and the director components under the Cartesian coordinate system are expressed as $0 = -[f_g]_V$ and $0 = -[f_g]_{Qjk}$, respectively. Where, $[f_g]_{Qjk}$ and $[f_g]_V$ represent the functional derivative of Q_{jk} and voltage V. By using these equations, we can calculate the components of the 3 by 3 Q tensor and voltages in each grid. The functional derivative equations are

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

$$[f_g]_S = -2(-\tfrac{1}{12}K_{11} + \tfrac{1}{4}K_{22} + \tfrac{1}{12}K_{33})Q_{jk,ll} - (K_{11} - K_{22}$$
$$-K_{33})Q_{jl,lk} - K_{24}Q_{jl,lk} + \tfrac{1}{4}(K_{33} - K_{11})(Q_{lm,j}Q_{lm,k}$$
$$-Q_{lm,l}Q_{jk,m} - Q_{lm}Q_{jk,ml} - Q_{lm,m}Q_{jk,l} - Q_{lm}Q_{jk,lm})$$
$$+2q_0K_{22}e_{jlm}Q_{mk,l},$$

$$[f_g]_V = -\tfrac{1}{2}e_0D_eV_{,j}V_{,k} \qquad (4)$$

$$[f_g]_T = \left(A_1 + A_2\frac{T}{T_{ni}}\right)Q\cdot Q + A_3Q\cdot Q\cdot Q + A_4Q\cdot Q\cdot Q\cdot Q,$$

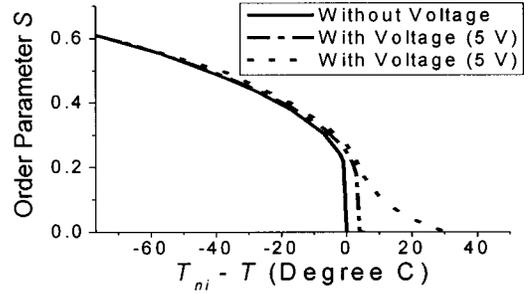$$Q_{jk,ll} = \frac{\partial}{\partial\ell}\left(\frac{\partial Q_{jk}}{\partial\ell}\right),$$

FIG. 1. 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.

where 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 different from each nematic 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. 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, 0.784, 0.61, and 1.474 J/C m^3, respectively, were determined. For the equilibrium state, the Q tensor and voltages in each grid should be recalculated in every time step until they exhibit stable response. We can achieve them by using the dynamic equation $\gamma(\partial Q_{jk}/\partial t) = -[f_g]_{Qjk}$. γ is rotational viscosity and we ignored bulk viscosity because have not considered flow effect. 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 $Q_{jk}^{-\tau+1} = Q_{jk}^{-\tau} + \Delta t[fg]_{Q_{jk}}/\gamma$. Using this equation, the Q-tensor components can be updated at each time step, so that the final value of the Q tensor is the equilibrium state. The order parameter S is related to the Q tensor in the equation by $S^2 = 1.5(Q \cdot Q)$ and we can get this simultaneously with the Q components.
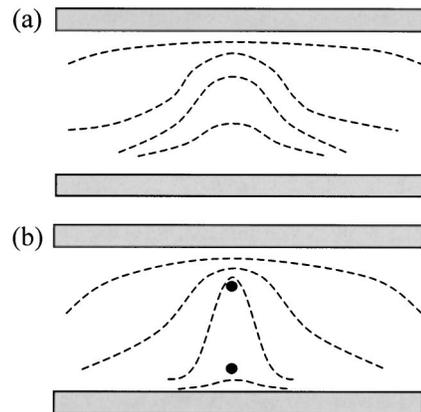

FIG. 2. Cartoons of the pincement phenomenon, which show the conversion of a reverse tilt wall to a pair of line defects (after de Gennes): (a) a reverse tilt wall and (b) a pair of line defects. The dashed lines represent the orientation of the LC director field. The two-circled areas in Fig. 3(b) represent the line defects.
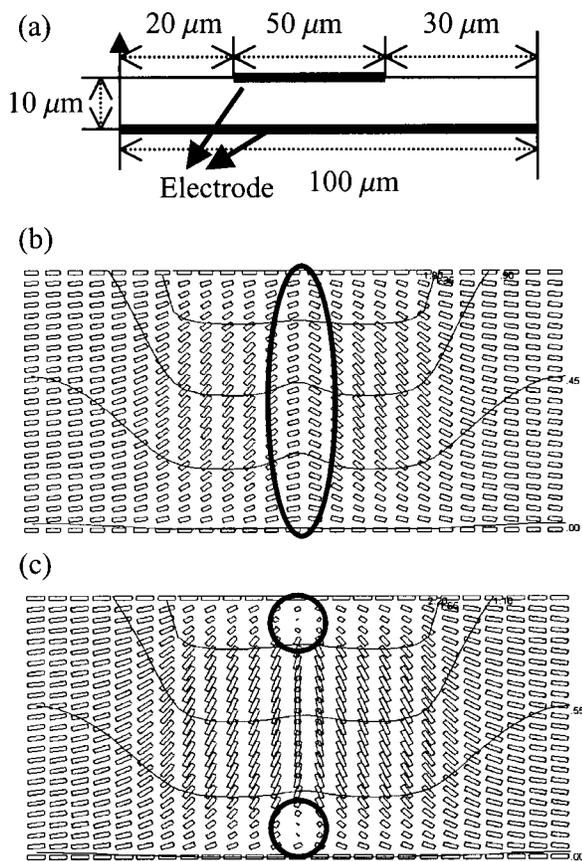
FIG. 3. Two-dimensional director calculations for the modeling of the LC director field that contains line disclinations pincement: (a) a simulated structure, (b) at 2 V, and (c) at 3 V. The calculated results are sampled to half. The solid lines represent equipotential lines. The electric field direction is normal to the equipotential line. The oval in Fig. 3(b) highlights the high elastic strain region where the pair of defects will nucleate. The circles in Fig. 3(c) highlight the line disclinations after they separated and moved toward the cell surfaces.

The Landau–de Genns's Q tensor has zero trace ($\Sigma Q_{ii}=0$) and it implies that LC director is a unit vector ($\Sigma n_i^2=1$). So, we need to normalize the calculated Q-tensor at every time step so that it is traceless and n is a unit vector. Typically, the condition of tracelessness is directly imposed when numerically determining the equilibrium value of the Q tensor.[5] However, we have found serious problems with this method when an electric field is applied. To maintain normalization using this method, the time steps must be kept extremely short. Therefore, the normalization that starts from the unit vector property is more appropriated for the physical and numerical situation. The normalization to gain a unit vector can be written simply as $n_i=n_i/|n_i|$. We can easily derive the normalization for the Q-tensor notation to be $Q_{ii}=(Q_{ii}-T_r/3)[S/(T_r+S)]$. This indicates that $\Sigma Q_{ii}=0$, and so this equation causes the Q tensor to be always traceless and the LC director n_i will have unit amplitude, however, we have found much larger time steps can be taken with this method.

Figure 1 shows 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.

To demonstrate the proposed method, we have compared calculated results with the diagrammatic prediction of de Gennes for the transition of a reverse tilt wall to a pair of disclination lines. de Gennes showed that at some voltage the transition should occur, but did not show its details. Figure 2 is an example of this phenomenon, so called the "pincement" of Bouligrand,[3] where a pair of disclination line ($m=-1/2$ and $m=+1/2$) is nucleated from a reverse tilt wall. In order to model the pincement, we calculated cell with two-dimentional patterned electrodes that has a 10 μm cell gap and is filled with the LC material ZLI-1565 as shown in Fig. 3(a). Figures 3(b) and 3(c) are the calculated results for Figs. 2(a) and 2(b), respectively. For the calculation, the number of calculated layers was set to 50×50 in the x and z directions. In the figure, length of the lines is proportional to amplitude of S. From the figures, we can see that the pair of defects originated in the middle of the LC layers because of symmetrical and nonuniform field distribution. By increasing the voltage, the orientation of the LC directors becomes more sharp like Fig. 3(b) and the defects separate to lower the strain distortion energy of the cell, so that the defects move to the surface of the cell. This process is consistent with the explanation for the pincement. Therefore, we confirmed that the proposed method can model the configuration of the LC director field including most of defects successfully. de Gennes mentioned that the size of the defect core might be approached to molecular dimensions.[3] However, the size of the region where the order parameter is not a constant, which is controlled by the temperature parameter A_1 to A_4 that was introduced earlier, is here set to larger values to allow visualization of the defect core.

In conclusion, a Q-tensor method for fast calculations of a liquid crystal director configuration containing the defects has been presented. The method is directly derivable from the Oseen–Frank free energy, is computationally simple, and allows for accurate modeling of defect nucleation and director field transitions between topologically inequivalent states.

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