Implementation of Q-Tensor Model into 3-D Finite Element Method (FEM) Numerical Solver

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Keywords : FEM, Q-Tensor, OCB, π-cell LCD

Abstract

In this paper, we report our successful implementation of Q tensor model in three-dimensional finite element method (FEM) simulator. The 3D-FEM Q tensor-model-based simulation revealed that the spaly-to-bend transition occurs only at 4 V while the vector-model based FEM solver provides an erroneous transition voltage of 8 V.

1. Objectives and Background

A mathematical simulator for liquid crystal displays (LCDs) is an important tool for research and development. To calculate a director configuration, it is necessary to express the free energy of the system. The Gibbs free energy is minimized, in the equilibrium state of the director with constant potential. It consists of elastic deformation terms and electric field terms. For the elastic term, Oseen-Frank elastic free energy, vector approach, is widely used. The Oseen-Frank vector approach requires less mesh points to assure numerically accurate results and stabilities. And it is fast method because its formulation is simple. Although it has many advantages, it is wrong method for director configurations of in LC cell. The nematic LC has quadrupole, that is to say, it has 'inversion symmetry'. Inversion symmetry means 'the n and –n equivalence' [1]. On the other hand, Landau-de Gennes's Q tensor approach requires more mesh points to assure numerically accurate results and stabilities. Owing to complicated formulation Q tensor approach is slow method. It has many disadvantages. Nevertheless, it satisfies the nematic LC's inversion symmetry. So Q tensor approach is considered to superior to vector approach recently. Dickmann has shown that Oseen-Frank vector approach be changed to Q tensor approach directly [2].

2. Mathematical Models

LC molecules which are elastic bodies have elastic force when disequilibrium state. This elastic force is defined elasticity theory which means elastic force vary in proportion to deformation rate. Equation (1) is Oseen-Frank elastic free energy density with the K24 term. The K24 terms can be omitted owing to the integration of K24 terms adds only a constant and doesn't affect the equilibrium configurations.

$$f_s = \frac{1}{2}K_{11}(\nabla \cdot \vec{n})^2 + \frac{1}{2}K_{22}(\vec{n} \cdot \nabla \times \vec{n})^2 + \frac{1}{2}K_{33}(\vec{n} \times \nabla \times \vec{n})^2$$
$$- \frac{1}{2}(K_{22} + K_{24})\nabla \cdot (\vec{n} \cdot \nabla \cdot \vec{n} + \vec{n} \times \nabla \times \vec{n})$$
$$- q_0 K_{22}(\vec{n} \cdot \nabla \times \vec{n}) \tag{1}$$

K is the elastic constants and K11, K22 and K33 are the splay, twist, and bend elastic constants, respectively. $\vec{n}$ is the director with unit length, and q0 = 2π/p0 is the chirality of the LC. Equation (2) is the Q tensor elastic free energy density.

$$f_s = \frac{1}{27}(k_{33} - k_{11} + 3k_{22})\frac{G_1^{(2)}}{S^2} + \frac{2}{9}(k_{11} - k_{22} - k_{24})\frac{G_2^{(2)}}{S^2}$$
$$+ \frac{2}{9}k_{24}\frac{G_3^{(2)}}{S^2} + \frac{2}{27}(k_{33} - k_{11})\frac{G_6^{(3)}}{S^3} + \frac{4}{9}q_0 k_{22}\frac{G_4^{(2)}}{S^2} \tag{2}$$

$$G_1^{(2)} = Q_{jk,l}Q_{jk,l}, \qquad G_2^{(2)} = Q_{jk,k}Q_{jl,l},$$
$$G_3^{(2)} = Q_{jk,l}Q_{jl,k}, \qquad G_4^{(2)} = \varepsilon_{jkl}Q_{jm}Q_{km,l},$$
$$G_6^{(3)} = Q_{jk}Q_{lm,j}Q_{lm,k} \tag{3}$$

with

$$Q_{jk} = \frac{S}{2}(3n_j n_k - \delta_{jk})$$

$$Q_{jk,l} = \frac{\partial Q_{jk}}{\partial l}, \dots \qquad j,k,l \in \{x,y,z\}. \tag{4}$$

Q is the tensor order parameter, and S is the scalar order parameter. ε_{ijk} is the Levi-Civita symbol ($\varepsilon_{123}=\varepsilon_{231}=\varepsilon_{312}=-1$, $\varepsilon_{132}=\varepsilon_{213}=\varepsilon_{321}=-1$, all other $\varepsilon_{ijk}=0$). δ_{jk} is Kronecker delta ($\delta_{jk}=1$, when j=k; otherwise $\delta_{jk}=0$). Dickmann has shown that Oseen-Frank vector approach be changed to Q tensor approach directly [3, 4].

3. Simulation Results and discussion

Figure 1 shows a splay to bend transition in OCB mode. The OCB cell was first proposed by Bos et. Al. in 1984 [5~7], having a fast relaxation time and a large cone of view. The OCB cell shows the splay state at lower voltages and the bend state at higher voltages. It is because the Gibbs free energy is minimized in the splay state when the applied voltage is low and it is minimized in the bend state when the applied voltage is high [8].
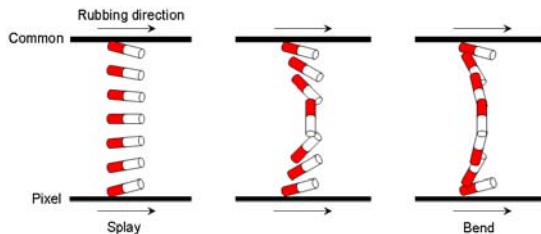

**Fig. 1. Splay to bend transition of the OCB cell**

Figure 2 shows the one-dimensional director configurations in OCB cell. Figure 2(a) represents applied voltages. The voltages increase from 0 [V] to 10 [V] and decrease 10 [V] to [0]. In Fig. 2(b), director configurations applying vector approach show splay to bend transition about 8 [v]. Because vector approach could not satisfy the inversion symmetry, director is opposite in the middle of the spaces; therefore it is stored high distortion energy. Thus it needs more electric energy than tensor approach. On the other hand, tensor approach satisfies the inversion symmetry. Because it has no distortion energy in the middle of the space, it shows splay to bend transition at lower voltages than vector approach. Figure 2(c) represents the director configurations applying tensor approach.
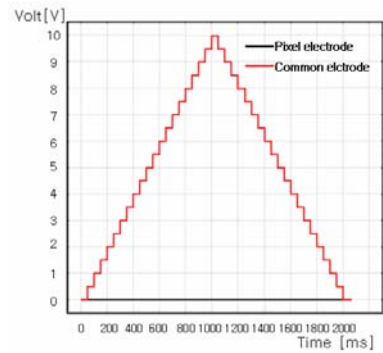
(a) Applied voltages
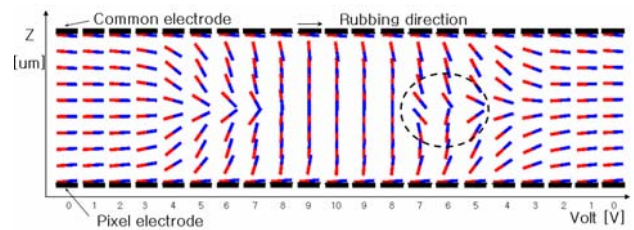
(b) Vector approach
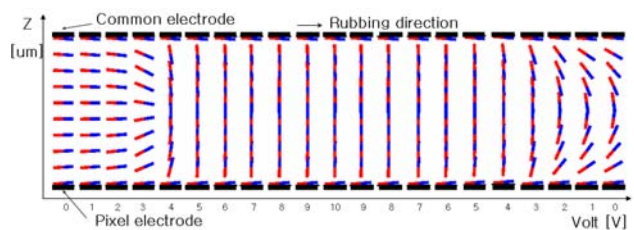
(c) Q tensor approach

Fig. 2. Calculated one-dimensional director configurations. (a) The graph shows the applied voltages. Vector and Q tensor approach is similar results when the voltage increases 10 [V] but it is different results when the voltage decreases 0 [V].

Figure 3 indicates our cell geometry used for the two dimensional director calculations. We also applied voltages which are same Fig. 2(a) in common electrode.
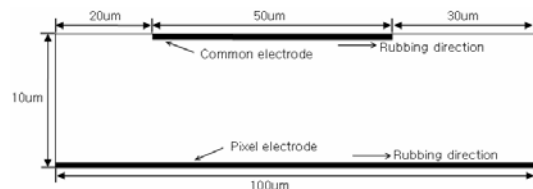

Fig. 3. The cell geometry used for the calculation.

(a) Vector approach at 3 [V]

(b) Q tensor approach at 3 [V]
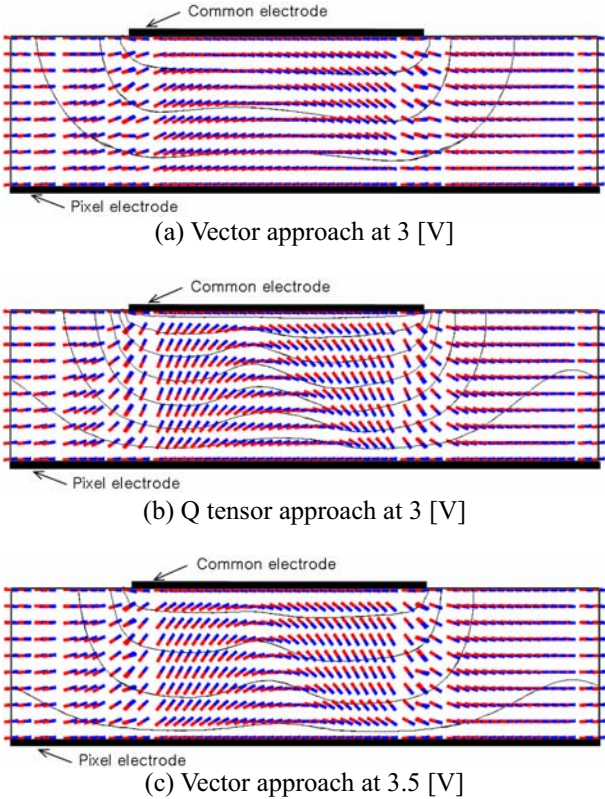

(c) Vector approach at 3.5 [V]

Fig. 4. Two-dimensional director configurations. They are applied voltages to increase from 0 [V] to 10 [V]. (a) and (b) are applied 3 [V] and (c) is applied 3.5 [V] in common electrode.

(a) Vector approach at 3 [V]

(b) Q tensor approach at 3 [V]
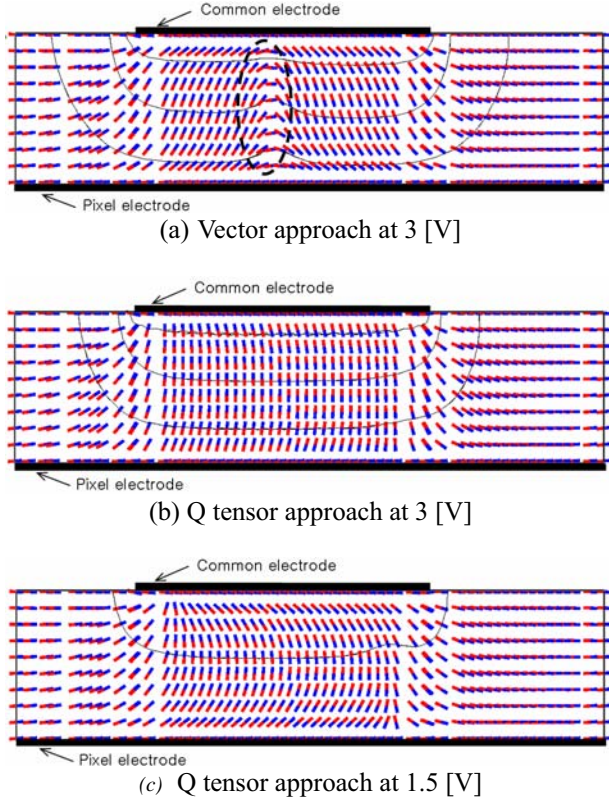

(c) Q tensor approach at 1.5 [V]

Fig. 5. Two-dimensional director configurations. They are applied voltages to decrease from 10 [V] to 0 [V]. (a) and (b) are applied 3 [V] and (c) is applied 1.5 [V] in common electrode.

Figure 4(a) and (c) are respectively applied 3 [V] and 3.5 [V] to increase voltages using vector approach and (b) is applied 3 [V] using tensor approach. In Fig. 4(a) and (b) shows vector approach is needed more voltage than tensor approach for splay to bend transition. But it is only needed more voltages, its director configurations are similar at the increasing voltages.

Figure 5(a) is applied 3 [V] to decrease voltages using vector approach and (b) and (c) are applied 3 [V] and 1.5 [V] using tensor approach. In Fig. 5(a) and (b) shows different direction configurations at the decreasing voltages in the abovementioned about it. We can also know that tensor approach has more relaxation time. Although Fig. 5(b) decreases the voltages more, the director configurations of vector approach and tensor approach are different configurations at decreasing voltages. We can know it to compare with Fig. 5(a) and (c). In Fig. 5(a), we can observe the director distortion in the center of the cell.

So far, we calculate one-dimensional and two-dimensional director conformation using three-dimensional simulator applying Q tensor approach. Our results are right to compare the previous papers [9]. These results verify our simulation.

Finally we calculated three-dimensional director configurations. Figure 6 shows our cell geometry. This cell is similar the cell of Fig. 3. We applied same voltage before simulation. And we investigate the director configuration at ABCD square. It is the center of the cell.
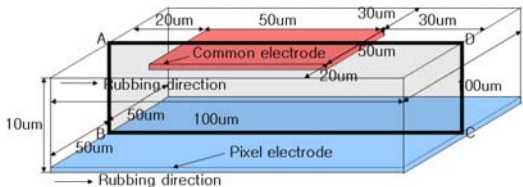

Fig. 6. The cell geometry used for the calculation.
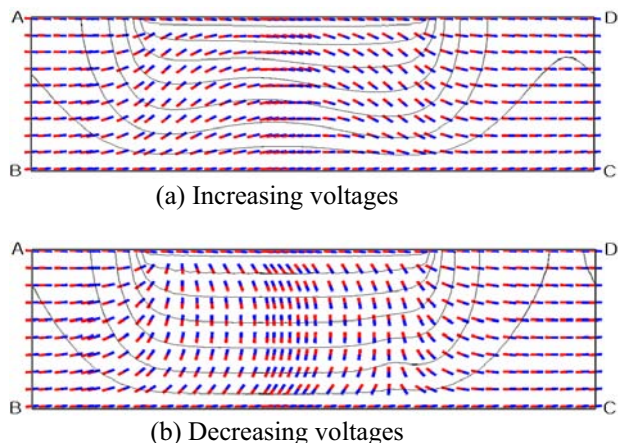
(a) Increasing voltages

(b) Decreasing voltages

Fig. 7. Three-dimensional director configurations. This is applied Q tensor approach. (a) is applied 3 [V] in common electrode when the voltage is increased. (b) is applied 3 [V] when the voltage is decreased.

Figure 7(a) is applied 3 [V] when the voltage is increased and (b) is applied 3 [V] when the voltage is decreased. It is similar to two-dimensional results because its cell structure is extended from 2D to 3D. Although our simulation cell is very simple, the results is very precise. Further we will calculate realistic cell structure. This simulator is very useful for it.

4. Conclusion

In this paper, we report our successful implementation of Q tensor model into three-dimensional FEM simulator for the first time.

The director response was carefully investigated between the vector model and Q tensor model. Our 3D-FEM simulation reveals that the dynamic response, especially during the recovery period, of the OCB mode requires Q tensor model for accurate estimation.

5. Acknowledgment

6. References

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