Comparative Study on Tensor and Vector Approaches for 3D-FEM Numerical Simulator

Sang Young Cho[1], Seung Soo Yang[1], Hyoung Jin Yoon[2], Tae Young Won[1]
[1]Dept. Electrical Engineering, Inha Univ., Incheon 402-751, Korea
TEL:82-32-860-7436, e-mail: csy@hsel.inha.ac.kr.
[2]Sanayi System Co., Incheon 402-711, Korea

Keywords : FEM,, OCB, Tensor

Abstract

We report our study on the implementation of Q tensor approach into three-dimensional finite element method (FEM) numerical solver. The comparative simulation results demonstrated the possibility of a different director configuration in between Q tensor method and vector method. The comparative study confirmed that Q Tensor implementation is more appropriate for OCB analysis than the vector method.

1. Introduction

With the development of LCD technology, the pixel structure becomes more complicated due to various electrode patterns and a lot of optical films. Computer simulation tools help the designer to understand the behavior of the directors in the cell. We can predict what problems might develop and how they can be solved by calculating the director configuration on the computer.

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. But, in case of 'the n and –n equivalence state' has inexact high distortion[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. But, Q tensor approach has that the sign of n is always cancelled out even when finite differences for the spatial derivatives are considered. So, Q tensor satisfies the nematic LC's inversion symmetry.[2]

2. Mathematical Models

We use director modeling to consider an OCB cell. OCB cell is a nematic liquid crystal display in which the molecular director bens symmetrically by 180^0 through the cell. The OCB cell has a unique characteristic of showing the splay state at lower voltages and the bend state at applied higher voltages[3]

Since these states are topologically different form each other, transition between the splay state and the bend state inevitably accompanies with bend nucleus.

Conventional OCB cell is never changed to bend state without bend transition core even after more than a critical voltage is applied to obtain uniform transition from splay to bend states, bend transition core must exist[4]. So we use the OCB cell for the comparing the characteristic of mathematical modeling.

Equation (1) is Oseen-Frank elastic free energy density with the K_{24} term. The K_{24} terms is related to surface anchoring energy. We can omit the K_{24} terms when strong anchoring energy state.

$$\begin{aligned} f_s = & \frac{1}{2}K_{11}(\nabla\cdot\vec{n})^2 + \frac{1}{2}K_{22}(\vec{n}\cdot\nabla\times\vec{n})^2 + \frac{1}{2}K_{33}(\vec{n}\times\nabla\times\vec{n})^2 \\ & -\frac{1}{2}(K_{22}+K_{24})\nabla\cdot(\vec{n}\cdot\nabla\cdot\vec{n}+\vec{n}\times\nabla\times\vec{n}) \\ & -q_0K_{22}(\vec{n}\cdot\nabla\times\vec{n}). \end{aligned} \quad (1)$$

K_{11}, K_{22} and K_{33} are the splay, twist, and bend elastic constants, respectively. N is the director with unit length, and $q_0 = 2\pi/p_0$ is the chirality of the LC.

Equation (2) is the Q tensor elastic free energy density which is the derived from Dickman[5].

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

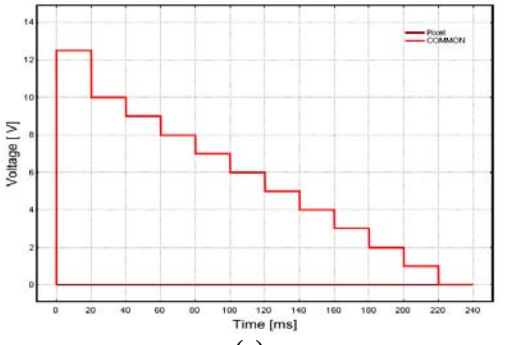
$$G_1^{(2)} = Q_{jk,l}Q_{jk,l}, \quad G_2^{(2)} = Q_{jk,k}Q_{jl,l},$$
$$G_3^{(2)} = Q_{jk,l}Q_{jl,k}, \quad G_4^{(2)} = \varepsilon_{jkl}Q_{jm}Q_{km,l},$$
$$G_6^{(3)} = Q_{jk}Q_{lm,j}Q_{lm,k} \quad (3)$$

With

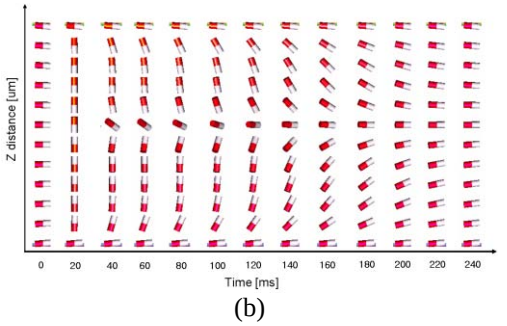
$$Q_{jk} = S(n_j n_k - \frac{\delta_{jk}}{3}), \quad Q_{jk,l} = \frac{\partial Q_{jk}}{\partial l} \quad (4)$$

Q means the Q tensor order parameter, and S means the scalar order parameter. The Levi-Civita symbol is $\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = -1$, $\varepsilon_{132} = \varepsilon_{213} = \varepsilon_{321} = -1$, all other $\varepsilon_{ijk} = 0$). δ_{jk} is Kronecker delta ($\delta_{jk} = 1$, when j=k; otherwise $\delta_{jk} = 0$).

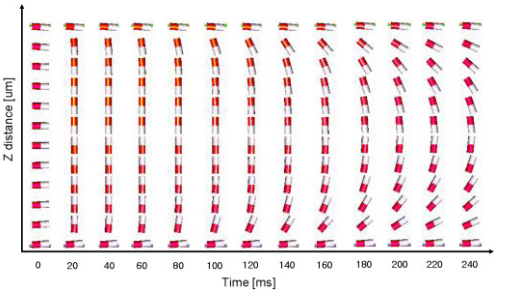
3. Simulation



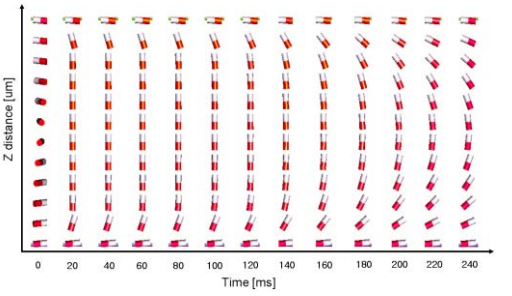
(a)



(b)



(c)



(d)

Fig. 1. The results of calculated director configurations. (a) shows the applied voltages. (b) vector approach for splay state (c) tensor approach for splay state (d) vector approach for 180° STN state.

We used the physical parameters of ZLI 1557 from Merck. The cell thickness was assumed to be 10um. And the cell size was 40um × 40um. Each case the applied field was turned on at time t = 0ms and off at t = 60ms.

In figure 1, we calculated the dynamic molecules of director configuration as a function of time for a pi-cell. We defined splay state which had the pretilt 5° of bottom and the pretilt -5° of top as shown in Fig.1 (b~c). And we defined 180 STN states which had the pretilt 5° of bottom and the pretilt 5° of top, azimuthal angle 180 of top in Fig.1 (d). We started the system in the splay state and applied 12.5 volts during 20ms[6]. And then we applied 10 volts and decreases voltage for 1V per 20ms.

When the field was switched off, the vector approach returned to the splayed configuration in Fig.1 (b). And director was opposite in the middle of the spaces during 40ms ~ 140ms in Fig.1 (b). It means that director in the middle of the space had high distortion energy. Therefore the vector approach gives an inexact high value of the elastic energy of the director configuration.

While the tensor approach transformed to the bend state in the Fig.1 (c). And the tensor approach had not

distortion in the middle spaces. It means that the middle spaces have the vector n and vector –n equivalence yields a low energy uniform director configuration. So in this simulation, the results of tensor approach have more reliable than the results of vector approach.

For the purpose of further development, we compared the results of tensor approach with the results of 180 STN states. In Fig.1 (d), the results of vector approach 180 STN state was mostly similar to the results of tensor approach in Fig.1 (c) except initial condition at time t = 0ms. So we extract the tilt angle from the vector approach for 180 STN state and Tensor approach for splay state.

TABLE 1. Extract to tilt angle data from cases which are vector approach for 180 STN state and tensor approach for splay state.

Depth (um)	Tensor 0(ms)	Vector 0(ms)	Tensor 20(ms)	Vector 20(ms)	Tensor 80(ms)	Vector 80(ms)	Tensor 240(ms)	Vector 240(ms)
0.91	4.24	5.07	87.60	61.45	78.74	58.84	21.39	20.04
1.82	3.32	5.08	89.67	88.61	86.59	85.91	39.28	37.02
2.74	2.41	5.07	89.94	89.94	88.99	88.93	55.07	52.83
3.66	1.49	5.04	89.98	89.95	89.68	89.74	69.06	67.57
4.57	0.58	5.01	89.99	89.97	89.92	89.95	82.02	81.46
5.49	-0.34	5.05	-89.99	89.96	-89.94	89.93	-85.44	85.02
6.40	-1.25	5.07	-89.97	89.91	-89.74	89.72	-72.69	71.23
7.32	-2.17	5.08	-89.91	89.80	-89.09	89.08	-59.02	56.75
8.23	-3.08	5.06	-89.61	89.13	-86.97	87.12	-43.82	41.30
9.15	-4.00	5.03	-87.95	79.99	-80.16	76.58	-26.57	24.78

Referring to Table 1, tilt angle of director was continuously change from bottom to top in case of tensor approach for splay state at t = 0ms. And tilt angle of director was mostly 5^{o} in case of vector approach for 180 STN state at t = 0ms. This is certifies that correctness of calculation for initial director condition in each cases. Both of all have similar director configuration at 240 ms. But, vector approach for 180 STN state has sudden change director configuration to top surfaces (61.45^{o} → 88.61^{o}) and bottom surfaces (89.13^{o} → 79.99) at 20ms in table 1. And this tendency has preserved for over 80ms. While the tensor approach for splay state has smoothly change director configuration from top surface to bottom surface during the same periods. So for the purpose of calculating OCB mode, tensor approach is more reliable than vector approach.

4. Conclusion

We investigated three cases having opposite regions due to the vector n and vector –n equivalence. Under the same condition, we found that there exists an overestimation of the elastic energy in the director configuration in the vector approach. Further, we compared tensor approach with 180 STN states which has very similar director configuration to tensor approach at 240ms. We found the abrupt change in director configuration from 20ms to 80ms in case of vector approach for 180 STN state. Therefore, tensor approach seems to be more reliable for the analysis of OCB mode.

5. Acknowledgement

This research was supported by the MIC(Ministry of Information and Communication), Korea, under the ITRC(Information Technology Research Center) support program supervised by the IITA(Institute of Information Technology Advancement) (IITA-2006-C109006030030).

6. References

1. J. E. Anderson, et al, Liq. Cryst., Vol. 28, No. 1, p109 (2001).
2. H. Mori, E. C. Gartland, Jr., J. R. Kelly, and P. J. Bo s, Jpn. J. Appl. Phys., Part 1 38, 135 (1999).
3. P.J Bos and K.R. Koehler, Mol. Cryst. Liq. Cryst. p329 (1984).
4. Jun Ho Park, et al. SID'06 Dig. p709 (2006).
5. T. Miyashita, et al.: Eurodisplay'93 Dig. p.149 (1993).
6. Korean Patent Publication No.10-2006-0039868
7. J.E .Anderson, P. Watson, and P.J. Bos, SID Symposium Digest of Technical Papers Vol. 30, p 198-201 (1999) .
8. G.-D. Lee, et al.: Phys. Rev. E 67, 041715 (2003)