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## Multidimensional Modeling of Liquid Crystal Director Field in the Patterned Vertical Aligned LC Cell Using the Fast Q-Tensor Method

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*In this article we model the liquid crystal director field in the Patterned Vertical Alignment (PVA) LC using the fast Q-tensor method, which can model multidimensional director configurations with defects in the liquid crystal director field. In this work we model the LC director field with same condition of the real cell using fast Q-tensor method. Different from the result of the 2 dimensional calculation, in case of 3 dimensional simulation result, the defect line from the phase transition on the slit is not occurred. Since the generated defects due to geometry of the slit disturbed the phase transition in the middle of slit. We modeled the defect nucleation from geometry of the slit and LC director field of the conventional PVA cell. As a result, we could calculate optical transmittance of the conventional PVA cell.*

**Keywords:** defect; fast Q-tensor; liquid crystal; PVA

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## 1. INTRODUCTION

Recently, Liquid Crystal Displays (LCDs) is considered as a leading candidate for next generation display devices. LCDs have the most superior characteristics such as thinness, light weight, and low power consumption. A PVA LC cell [1] is one of the most common modes using a multi-domain effect for high optical performance LC cell with wide viewing angle and high contrast ratio. In general, however, LC cells using multi-domain effect for wide viewing characteristic show relatively low transmittance because non-uniform voltage for the multi-domain effect can make the active area of the PVA cell have reverse tilt domain, so that defects can occur in the active area. Therefore, the defect can decrease the optical transmittance.

In the conventional PVA LC cell, we have found 3 positions where defects occurred in the active area by applying the voltage and we modeled each cases of the defect by using the fast Q-tensor method [2]. Finally, we could calculate optical transmittance of the PVA cell. In this paper, we also compare the result of the modeling for LC configuration with that by using vector method.

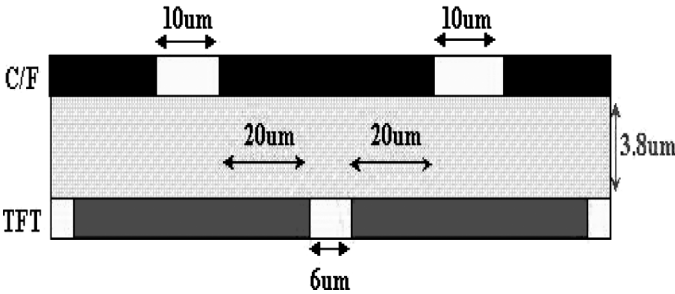
## 2. SIMULATION RESULTS AND ELECTRO-OPTIC CHARACTERISTIC OF CONVENTIONAL PVA CELL

### 2.1. 2 Dimensional Simulation Results

The fast Q-tensor method was used because it can calculate both the normal behavior of the LC director and the defect. The ideal of 2 dimensional PVA modeling condition, which is no disturbance of the structure on the edge, we can observe the difference of calculation results between the vector method and the fast Q-tensor method. As an example, Figure 2, shows the difference calculation results of two methods. Using the geometry shown in Figure 1.

Figure 2, shows that in this geometry. In the Cartesian vector representation, the discretized free energy expression gives different free energies for  $n$  and  $-n$  [3,4]. In real nematics, however,  $n$  and  $-n$  are equivalent and should give the same torque and the same free energy. The Q-tensor representation always incorporates the multiplication of two  $n$ 's [5]. This means that the sign of  $n$  is always cancelled out even when finite differences for the spatial derivatives are considered.

Figure 2(a,b) shows that the cross sectional view and top view of 8th layer each calculation method. The applied voltage is 8 V. We can observe the difference of director configuration of the middle of the slit area. Figure 2(a), the reverse tilt wall make the directors



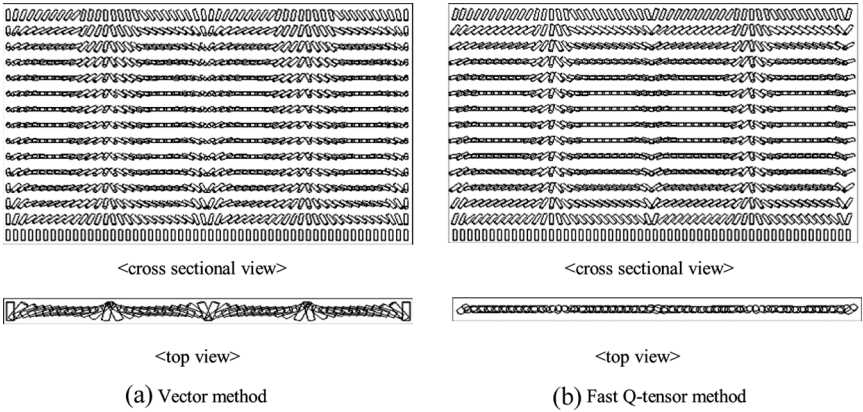
**FIGURE 1** The cell geometry used for the calculation.

configuration splay state. However, Figure 2(b), the phase transition occurred in the middle of the slit area.

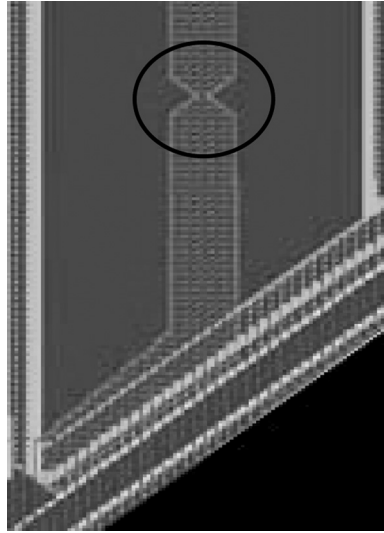
**2.2. 3 Dimensional Simulation Results**

The conventional PVA has 3 dimensional structure. As a results, the edge effect the director field of the slit area. We simulated the 3 dimensional LC modeling of conventional PVA's structure. And we observe that the edge effect distrurb the phase transition on the middle of slit area and generate another defect line moving to the active area.

Figure 3 shows the conventional structure of the slit in the PVA cell which includes defect trap in the center of the slit. In general, the conventional PVA cell without defect trap in the center shows very



**FIGURE 2** Calculation results for different method in a two-dimensional PVA cell.

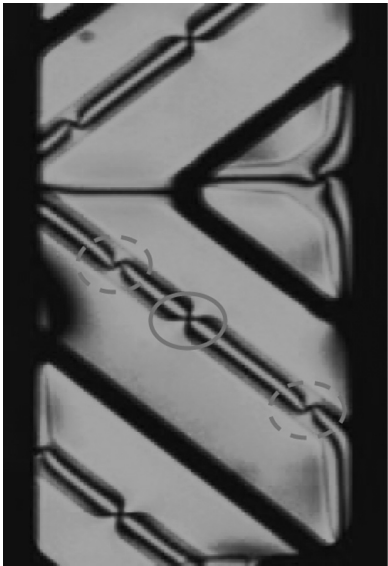


**FIGURE 3** The conventional structure of the PVA cell. Solid circle represents the defect trap in the center of the slit.

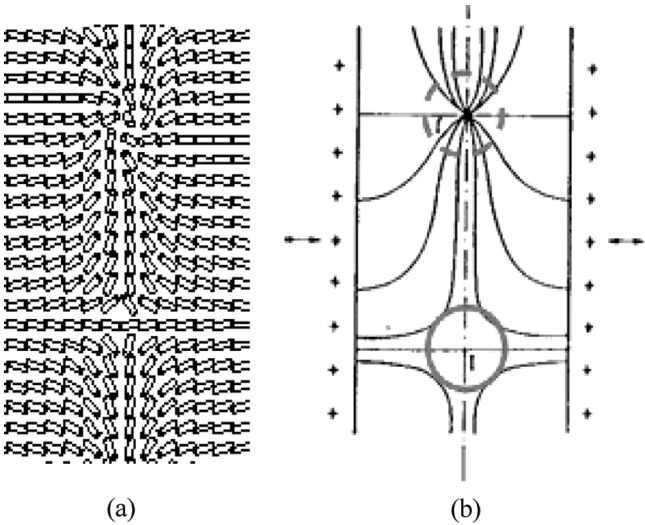
unstable dynamic behavior because the generated defect due to the competition of the strain energy from slit edge move along the slit by applying the voltage. Therefore, defect trap as shown in Figure 3 can prevent the defect from moving along the slit by applying the voltage.

On the contrary, however, the defect trap in the center of the slit can generate another defect as shown in Figure 4. Figure 4 shows the generated defect cores on the slit of the conventional PVA LC cell. In the figure, we can find 2 positions of the defect cores on the slit. In the Figure 4, solid circle represent defect generated by defect trap in the center of the slit and dotted circle represent the defect area which are induced by non-uniform voltage distribution around edge of the slit and defect trap.

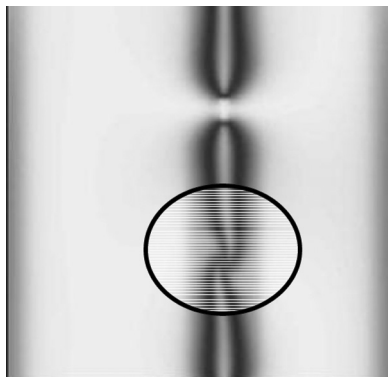
Figure 5(a) shows the 3-dimensional modeling of the LC director field on the slit. The director configuration in the solid circle represents the generated defect by defect trap in the center of the slit and that in the dotted circle represents the defect core due to the competition of the strain energy by the edge of the slit and the defect trap of the center. In the figure, we can assume that the LC director orientation due to the edge and the orientation due to the defect trap in the center are opponent along the slit as shown in Figure 5(a),



**FIGURE 4** Shows the generated defect cores on the slit of the conventional PVA LC cell.



**FIGURE 5** 3-dimensional LC director modeling of the PVA LC cell and cartoon of the orientation of the LC director.



**FIGURE 6** Calculated optical transmittance using the results of the fast Q-tensor method.

so that another can be generated. Figure 5(b) shows the cartoon of the modeling of the singular point for the Figure 5(a) [6]. The line in the Figure 5(b) represents the LC orientations. In the figure, we assume that the defect has Frank index ( $\pm 1/2$ ) with strength ( $\pm 1$ ).

Figure 6 shows that the 3 dimensional calculated optical transmittance with applying 8 V. The solid circle indicated the generating the defect core due to the edge structure and defect trap shape. Finally, we can calculate optical transmittance of defect in conventional PVA cell with 3 dimensional fast Q-tensor modeling.

### 3. CONCLUSION

In this article we modeled defect nucleation in the active area of the PVA cell. In order to model the defect as well as LC director configuration, we applied fast Q-tensor method, which can calculate scalar order parameter  $S$  in addition to director orientation  $n$ , to the modeling. Therefore, this article will also show the comparison of the result of the fast Q-tensor method and that of the vector method. The exact modeling using the tensor method will successfully calculate optical transmittance of the PVA cell.

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