P-162: Three-dimensional Molecular Director Simulation within a Unit Pixel of TFT-LCDs including Floating Electrodes

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Abstract

In this study, we presented a novel method to calculate unknown voltages on the floating electrodes introduced in a unit pixel of TFT-LCDs using three-dimensional molecular director simulation. For the simulation of the potential distribution profiles generated under the influence of the floating electrodes, we used the floating boundary condition on the surface enclosing the floating electrodes. The constraint for the floating boundary condition was derived from the charge neutrality condition about the floating electrodes disconnected from voltage sources. For the pixel with the floating electrodes patterned between the pixel and the data electrodes, we simulated the molecular director and the potential distribution in three-dimension, and then observed the location of the disclination lines around the edge of the pixel electrode. As a result, it was revealed that the floating electrodes significantly affect the electro-optical characteristics such as the location of the disclination line.

1. Introduction

Recently, in designing a unit pixel of thin film transistor liquid crystal displays(TFT-LCDs), the application of floating electrodes disconnected from any voltage sources has been gradually increased [1]. These floating electrodes are used for the purposes of not only blocking the obliquely incident light between the pixel and the data electrodes but also controlling the orientation of the liquid crystal molecules within the pixel. However, since the most reports, related to the three-dimensional simulation useful for the optimal design of the unit pixel of TFT-LCDs, have not explained the boundary conditions about the floating electrodes. Therefore, it is impossible to predict the potential distribution profiles and their corresponding molecular director profiles and to analyze the effects to the electro-optical characteristics on the floating electrodes introduced in the unit pixel of TFT-LCDs.

In this study, we present a novel method to calculate unknown voltages induced to the floating electrodes and their corresponding potential distribution profiles within the unit pixel of TFT-LCDs by using three-dimensional molecular director simulation. For the simulation of the potential distribution profiles generated under the influence of the floating electrodes, we use the floating boundary condition on the surface enclosing the floating electrodes. The constraint for the floating boundary condition is derived from the charge neutrality condition about the floating electrode disconnected from the voltage sources. The dynamic deformation profiles of the liquid crystal molecules are obtained three-dimensionally from the Ericksen-Leslie theory with Gibbs free energy density of liquid crystals [2]. As a numerical technique, we use finite difference method (FDM) on the rectangular and homogeneous grid due to the non-linearity of the governing equations [3]. For the pixel with the floating electrodes patterned between the pixel and the data electrodes, we simulate the dynamic behavior of the molecular director profiles and their corresponding optical transmission profiles, and then observe the location of the disclination lines around the edge of the pixel electrode to investigate the effect to the electro-optical characteristics on the floating electrodes.

2. Basic Concept of Modeling

To analyze the dynamic behaviors of nematic liquid crystals, we use the Erickson-Leslie theory, neglecting the inertial momentum of the molecules [2]. Applying the Gibbs free-energy density, f_g, to the Erickson-Leslie theory, we obtain

$$\gamma \frac{\partial}{\partial t} n_i = -[f_g]_{n_i} + \lambda n_i, \qquad i \in \{x, y, z\}, \tag{1}$$

where γ is the rotational viscosity, n_i is the cartesian component of the molecular director $\boldsymbol{n}(t, x, y, z)$, λ is a Lagrange multiplier introduced to maintain the director as a unit vector $|\boldsymbol{n}| = 1$, and $[f_g]_{n_i}$ is the Euler-Lagrangian equation defined by

$$[f_g]_{n_i} = \frac{\partial f_g}{\partial n_i} - \frac{d}{dx}\left(\frac{\partial f_g}{\partial n_{i,x}}\right) - \frac{d}{dy}\left(\frac{\partial f_g}{\partial n_{i,y}}\right) - \frac{d}{dz}\left(\frac{\partial f_g}{\partial n_{i,z}}\right). \tag{2}$$

Here, a comma followed by the suffixes x, y, or z denotes partial differentiation with respect to the x-, y-, or z-axis. The Gibbs free-energy density f_g is given as $f_g = f_s - f_e$, where f_s and f_e stand for the strain energy density and the electric energy density, respectively. The strain energy density can be expressed as

$$f_s = (-\frac{K_{11}}{12} + \frac{K_{22}}{4} + \frac{K_{33}}{12})G_1^{(2)} + (\frac{K_{11} - K_{22}}{2})G_2^{(2)} + (\frac{K_{33} - K_{11}}{4})G_6^{(3)} + q_0 K_{22} G_4^{(2)} \quad (3)$$

under an assumption that the surface term can be neglected [2]. We represent the strain energy density in a tensorial form to keep the equivalence of the director $\boldsymbol{n}$ and its opposite $-\boldsymbol{n}$ for nematic liquid crystals. In Eq. (3), K_{11}, K_{22}, and K_{33} represent the splay, the twist, and the bend elastic constants of the liquid crystals, respectively, and q_0 stands for the chirality of the liquid crystals. The G's are represented as

$$G_1^{(2)} = Q_{ij,k}Q_{ij,k} \ , \ G_2^{(2)} = Q_{ij,j}Q_{ik,k} \ ,$$
$$G_4^{(2)} = e_{ijk}Q_{il}Q_{jl,k} \ , \ G_6^{(3)} = Q_{ij}Q_{kl,i}Q_{kl,j} \ , \quad (4)$$

where the convention of summing over repeated indices is used. e_{ijk} is a permutation symbol, and the order tensor, Q_{ij}'s, is expressed as $Q_{ij} = n_i n_j - \delta_{ij}/3$ for the director $\boldsymbol{n}$. Here, we have assumed a perfect ordering of molecules with respect to the director in a differential volume. The electric energy density, f_e, is given as follows [2]:

$$f_e = \frac{1}{2}\varepsilon_o \phi_{,l} \varepsilon_{lm} \phi_{,m} \ , \quad (5)$$

where $\phi(x, y, z)$ is the potential distribution under a given driving voltage. ε_o is the permittivity of free space. ε_{lm} is the dielectric tensor of liquid crystals expressed as $\varepsilon_{lm} = \varepsilon_\perp \delta_{lm} + (\varepsilon_\parallel - \varepsilon_\perp) n_l n_m$, where $\varepsilon_\parallel$ and $\varepsilon_\perp$ are the parallel and the perpendicular dielectric constants of the liquid crystals, respectively. By substituting Eqs. (3) and (5) into Eq. (1), we get the dynamic equation of continuum theory for the director as follows [3]:

$$\gamma \frac{\partial n_i}{\partial t} = \{\frac{1}{3}(-K_{11} + 3K_{22} + K_{33})(n_j Q_{ji,ll}) + (K_{11} - K_{22}) n_j (Q_{il,lj} + Q_{jl,li}) + (\frac{K_{33} - K_{11}}{2}) n_j \times [2Q_{lm,m}Q_{ji,l} + 2Q_{lm}Q_{ji,lm} - Q_{lm,i}Q_{lm,j}] + 2q_0 K_{22} n_j (e_{iml}Q_{lj,m} + e_{jml}Q_{li,m}) + \varepsilon_o(\varepsilon_\parallel - \varepsilon_\perp) n_j \phi_{,j}\phi_{,i}\} + \lambda n_i, \quad (6)$$

where the electric potential distribution $\phi(x, y, z)$ can be obtained by computing the following Laplace equation derived from Maxwell's equation:

$$(\varepsilon_{ij}\phi_{,j})_{,i} = 0 . \quad (7)$$

Calculating the director and the potential distributions from Eqs. (6) and (7) is a highly complicated problem due to the dielectric anisotropy of liquid crystals and to the resultant coupling between the director and the electric field. To obtain the director distribution profile, we have to simulate Eqs. (6) and (7), which are coupled to each other by the director and the potential. As the equations are highly nonlinear, we adopt an iterative procedure separated in two steps as illustrated in Figure 1. First, we alternate between the solution for the potential while assuming a given director distribution and the solution for the director when the potential distribution is known until the iterative process reaches a steady state.

Now, we will describe a way to obtain the potential distribution profile within the calculation domain including the floating electrodes. As for the calculation of the potential profiles for various electrode such as pixel, common, data, and gate electrodes in the unit pixel of TFT-LCDs, Dirichlet boundary conditions have been introduced. However, for the floating electrodes, we have to consider floating boundary condition in company with other various boundary conditions. Related to the floating boundary condition, a constraint to obtain the potential distribution profile can be established by follows.

First of all, in the static condition, the surface of a floating electrode is considered as an equi-potential surface with a potential value of an unknown voltage V_f induced by the other driving voltages. Moreover, because the floating electrodes are not connected to any other voltage sources, there are no incoming or outgoing charges on the surface of the floating electrode. Therefore, the total charge induced on the floating electrode equals to always zero. From this, we can obtain the following equation of constraint related to the floating electrode.

$$\oint_{S_{FC}} \bar{D} \cdot d\bar{s} = -\oint_{S_{FC}} \varepsilon_r \varepsilon_0 (\nabla V) \cdot d\bar{s} = 0 \quad (8)$$

Here, S_{FC} represents the surface of floating electrode, ε_0 and ε_r are the dielectric constant of free space and relative dielectric constant around the floating electrode, respectively. $V(x, y, z)$ is the potential distribution profile within the calculation domain, as mentioned previously. Hereupon, since $D(x, y, z)$ satisfying the equation (8) depends on the unknown voltage of floating electrode V_f and potential distribution profile $V(x, y, z)$ around the floating electrode, we simulated numerically the potential distribution profile by successive over relaxation (SOR) method with the unknown voltage on the floating electrode for the given constraint of equation (8).

3. Results and Discussion

To investigate the effect to the electro-optical characteristics on the floating electrode introduced in the unit pixel of TFT-LCDs, we patterned the floating electrodes between the pixel and the data electrodes on the substrate where the TFTs are prepared. Figure 2 represents the three-dimensional structure of the various

electrodes together with the floating electrodes around the TFTs used in the simulation. Since the structures around the TFTs are very complex with the multiple electrodes, we reduced the calculation domain to a region around the TFTs surrounded by the neighboring four pixels, for the intensive simulation. The floating electrodes are overlapped with the pixel electrode as much as 3 μm width. Owing to the periodic boundary condition assumed here, the floating electrodes near the upper and the lower right pixels are considered as the same electrodes having the same voltage of V_{f1}. This is identical to the floating electrodes near the upper and the lower left pixel with the voltage on the floating electrodes of the value V_{f2}.

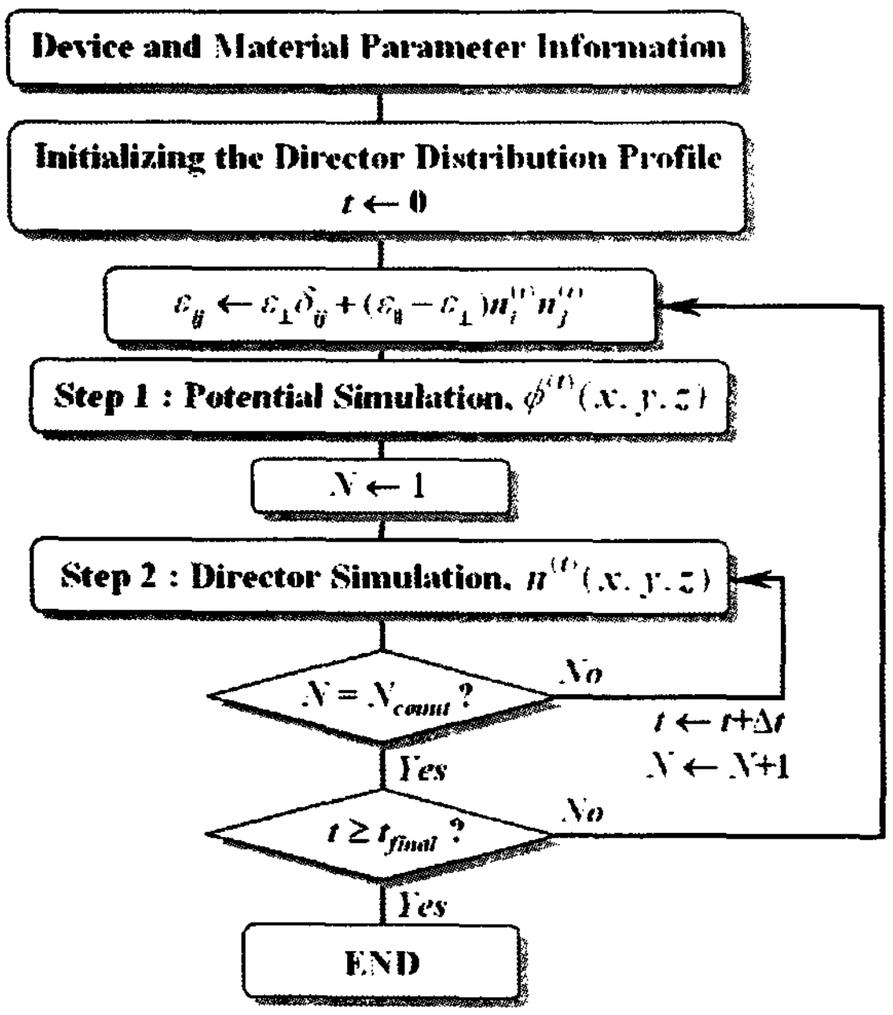


Figure 1. Iterative simulation procedure to obtain the director and the potential distribution profiles. Iteration between step 1 and step 2 is performed until a steady state of the director and the potential distributions is reached. Potential distribution profiles are simulated every 0.5 ms under the conditions of a numerical time step $\Delta t = 0.025\,ms$ and $N_{count} = 20$.

Figure 3 shows the voltages on each floating electrodes, V_{f1} and V_{f2} for solving the potential distribution with the floating electrodes under a fixed director profile and the variations of the solution for V_{f1} and V_{f2} as a function of time after the pixel voltage is applied. The pixel, the gate, the data, and the common electrodes are biased at 5 V, -8 V, 0.1 V, and 0 V, respectively. As shown in Figure 3 (a), the voltage on the floating electrodes converges well to their solution for each iteration step with the potential distribution profile to be solved. Moreover, in Figure 3 (b), V_{f1} and V_{f2} decrease slightly to finite value as a lapse of time because the dynamic motion of the molecular directors affects the effective dielectric constant of the liquid crystal layer.

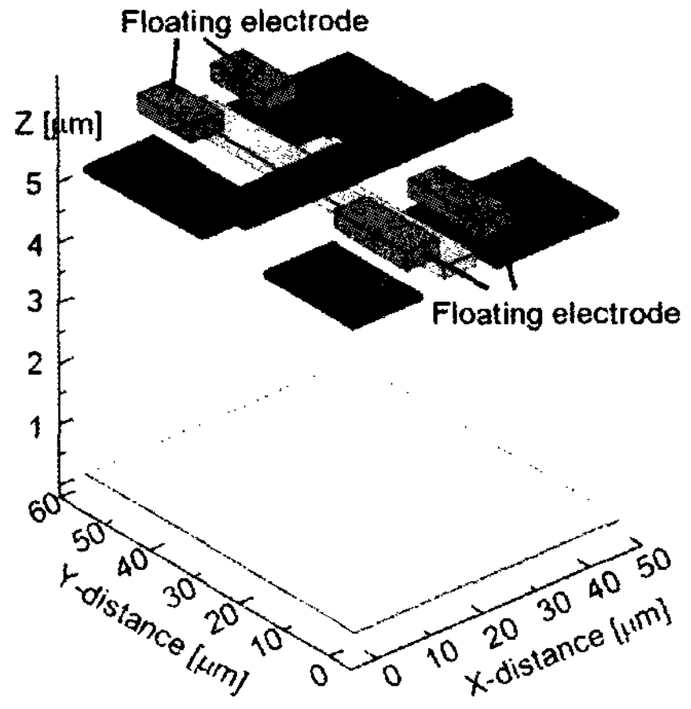
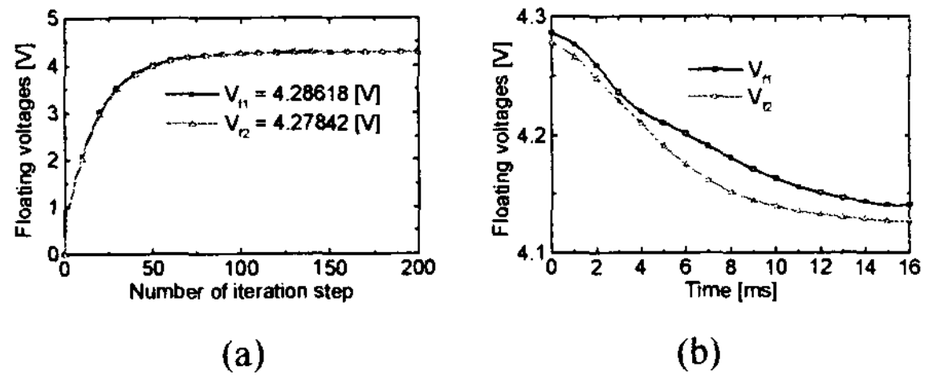


Figure 2. The three-dimensional structure of various electrodes together with the floating electrodes between the pixel and the data electrodes around the TFTs.

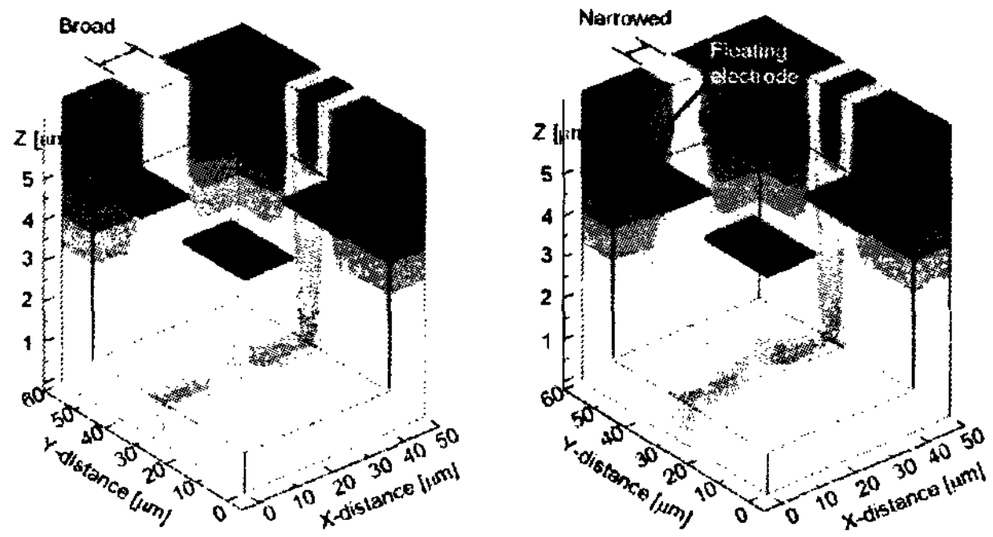


(a) (b)

Figure 3. (a) Convergences of the voltages on the floating electrodes for each iteration steps. (b) Variations of the voltages on the floating electrodes as a function of time.

Figure 4 depicts the three-dimensional equi-potential contour according to the absence and the presence of the floating electrodes. The lateral fields around the edge of the pixel electrodes become smaller due to the influence of the floating electrodes. From the saturated molecular director profiles, we observed the location of the disclination lines around the edge of the pixel electrode.

The optical transmission profiles along the cross section at $y = 50$ μm are plotted in Figure 5. Due to the floating electrodes between the pixel and the data electrodes, the location of the disclination line moves right to 1.3 μm compared with that of the structure which the floating electrodes are absent. From the results, it is revealed that the floating electrodes significantly affect the electro-optical characteristics such as the location of the disclination line. Therefore, it is expected that the proposed method is very useful for designing the unit pixel of TFT-LCDs including the floating electrodes.



(a) (b)

Figure 4. The equi-potential contours around the TFTs within the calculation domain.

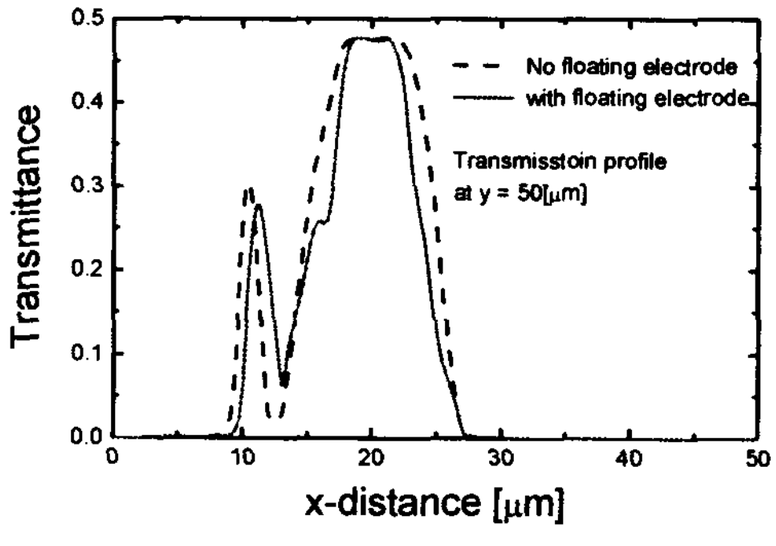


Figure 5. Optical transmission profiles at $y = 50$ μm as a function of the distance in x-direction. The peak position of the disclination line moves to 1.3 μm by the floating electrodes between the pixel and the data electrodes.

4. Conclusion

In the three-dimensional molecular director simulation of the TFT-LCDs equipped with the various floating electrodes, we presented a novel method to calculate the unknown voltages induced to the floating electrodes and their corresponding potential distribution profiles within a calculation domain. For the simulation of the potential distribution profiles generated under the influence of the floating electrodes, we used the floating boundary condition on the surface enclosing the floating electrodes. The constraint for the floating boundary condition is derived from the charge neutrality condition of the floating electrode. The dynamic deformation profiles of the liquid crystal molecules are obtained three-dimensionally from the Ericksen-Leslie theory with Gibbs free energy density of liquid crystals. As a numerical technique, we used FDM on the rectangular and homogeneous grid due to the non-linearity of the governing equations. For the pixel with the floating electrodes patterned between the pixel and the data electrodes, we simulated the dynamic behavior of the molecular director and their optical transmission profile, and then observed the location of the disclination lines. From the results, we confirmed that the floating electrode significantly affects the location of the disclination line. Therefore, it is expected that the proposed method is very useful for the design of a pixel of TFT-LCDs equipped with the floating electrodes.

5. Acknowledgments

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6. References

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