Comparisons between the Vector and Tensor Approaches for the 3-Dimensional Director Simulation of Liquid Crystal Displays

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Abstract

In this paper, we investigated dynamic behaviors of liquid crystal director profiles by simulating two different modeling equations based on vectorial and tensorial approaches. By performing 3-dimensional simulation for a unit pixel, we found that the simulation results from the each of modeling equations lead to different motional behaviors of liquid crystal directors around the disclination line. This is due to the fact that the vectorial approach has a physically meaningless sign of liquid crystal director $\vec{n}$. Consequently, it is clarified that the tensorial approach gives more realistic behaviors for the rotation of the directors around the disclination line when the voltages were removed since it maintains nematic symmetry that gives an equivalence of $\vec{n}$ and its opposite $-\vec{n}$.

1. Introduction

As the application of liquid crystal displays (LCDs) have expended to various ranges, the modeling and simulation of liquid crystals are becoming an essential problem in designing and optimizing the electro-optical characteristics of LCDs. As a results of a great efforts on the modeling and simulation of liquid crystals, many simulation of the 3-dimensional director deformation profiles have been performed extensively.

However, the previous works are concerned only to the calculation of the director deformation profiles of liquid crystals, and the works can be hardly found which are related to the physical and mathematical study on the comparisons between the modeling approaches which called the vector and tensor approaches. Therefore, we investigated dynamic behaviors of director deformation profiles of liquid crystals by simulating two different modeling equations based on vectorial and tensorial approaches. We used finite difference method (FDM) as a numerical technique, because it is useful to the complex governing equations and the structure used in this simulation.

By performing 3-dimensional simulation for a unit pixel, we found that the simulation results from the each of modeling equations lead to different motional behaviors of liquid crystal directors around the disclination line. This is due to the fact that the vectorial approach has a physically meaningless sign of liquid crystal director $\vec{n}$. Therefore, it is clarified that the tensorial approach gives more realistic behaviors for the rotation of the directors around the disclination line when the voltages were removed since it maintains nematic symmetry that gives an equivalence of $\vec{n}$ and its opposite $-\vec{n}$.

2. Theory

To obtain the dynamic motion of the 3-dimensional director deformation of liquid crystal displays, we used the Ericksen-Leslie theory neglecting the inertial moment and flow effect of liquid crystal molecules. Applying the Gibbs free energy density F_G to the theory, we obtain the governing equation for the dynamic motion of liquid crystal director $\vec{n}(x, y, z : t)$.

$$\gamma \frac{\partial n_i}{\partial t} = -\left[F_G \right]_{n_i} + \lambda n_i \qquad (1)$$

where n_i is the cartesian component of the director which is defined as the average molecule direction at some local position (x, y, z). γ is a rotational viscosity and λ is Lagrange multiplier introduced to

maintain the director to be a unit vector $|\vec{n}| = 1$.

According to the Oseen-Frank elastic theory, the Gibbs free energy density is written in terms of director $\vec{n}$, which is generally known as a vectorial form.

$$F_G = \frac{1}{2}K_{11}(\nabla \cdot \vec{n})^2 + \frac{1}{2}K_{22}(\vec{n} \cdot \nabla \times \vec{n} + q_0)^2 + \frac{1}{2}K_{33}|\vec{n} \times \nabla \times \vec{n}|^2 - \frac{1}{2}\phi_{,i}\varepsilon_0[\varepsilon_\perp \delta_{ij} + (\varepsilon_\parallel - \varepsilon_\perp)n_i n_j]\phi_{,j} \quad (2)$$

Here, K_{11}, K_{22} and K_{33} represent splay, twist and bend elastic constant of the liquid crystals, $\varepsilon_\parallel$ and $\varepsilon_\perp$ are parallel and perpendicular dielectric constants of liquid crystals, respectively. $\phi(x,y,z)$ is the electric potential profile at the inner side of a pixel formed by the pixel and neighboring electrode voltages. However, the vectorial form derived from the Oseen-Frank elastic theory cannot preserve the nematic symmetry, that is, the equivalence of the director $\vec{n}$ and $-\vec{n}$. Therefore, the vectorial form has the physically meaningless sign that is incorrect modeling for the liquid crystal director. To avoid the physically meaningless sign, there is an alternative way describing the Gibbs free energy density in terms of the order tensor $Q_{ij} = n_i n_j - \frac{1}{3}\delta_{ij}$. This is known as the tensorial form that the nematic symmetry is taken into account.

$$F_G = \left(-\frac{K_{11}}{12} + \frac{K_{122}}{4} + \frac{K_{33}}{12}\right)Q_{ij,k}Q_{ij,k} + \left(\frac{K_{11} - K_{22}}{2}\right)Q_{ij,j}Q_{ik,k} + \left(\frac{K_{33} - K_{11}}{2}\right)Q_{ij}Q_{kl,i}Q_{kl,j} + q_0 K_{22} e_{ijk} Q_{il}Q_{jl,k} - \frac{1}{2}\varepsilon_0\bar{\varepsilon}\phi_{,j}\phi_{,j} - \frac{1}{2}\varepsilon_0(\varepsilon_\parallel - \varepsilon_\perp)\phi_{,j}\phi_{,k}Q_{jk} \quad (3)$$

By substituting energies based on the vectorial form in equation (2) to the equation (1), and the tensorial form in equation (3) to the equation (1), we can obtain two different director equation of motion for the liquid crystals, named as vectorial form and tensorial form. As shown in equation (2) and (3), because the director equation of motion is concerned with the electrical energy density, we must simulate the potential profile and then simulate the director equation of motion simultaneously, as the lapse of time. The potential distribution can be obtained by simulating the generalized Laplace equation for an inhomogeneous and electrically anisotropic medium as follows.

$$(\varepsilon_{lm}\phi_{,m})_{,l} = 0, \quad \varepsilon_{lm} = \varepsilon_\perp \delta_{lm} + (\varepsilon_\parallel - \varepsilon_\perp)n_l n_m \quad (4)$$

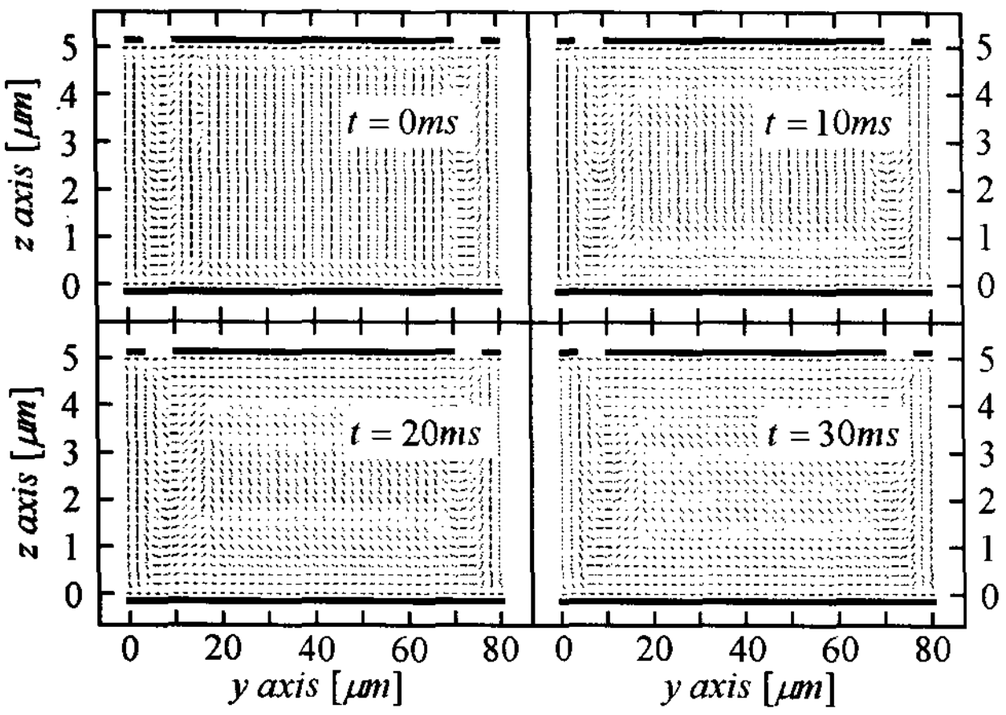
3. Results and Discussion

To compare the relaxation behaviors of directors simulated from the vectorial and tensorial approach, we applied a voltage to the pixel electrode to obtain the director deformation profiles of liquid crystals including the disclination line located between the normal and reverse tilt domains. After the voltage is removed from this saturation state, the directors become to relax freely with the lapse of time.

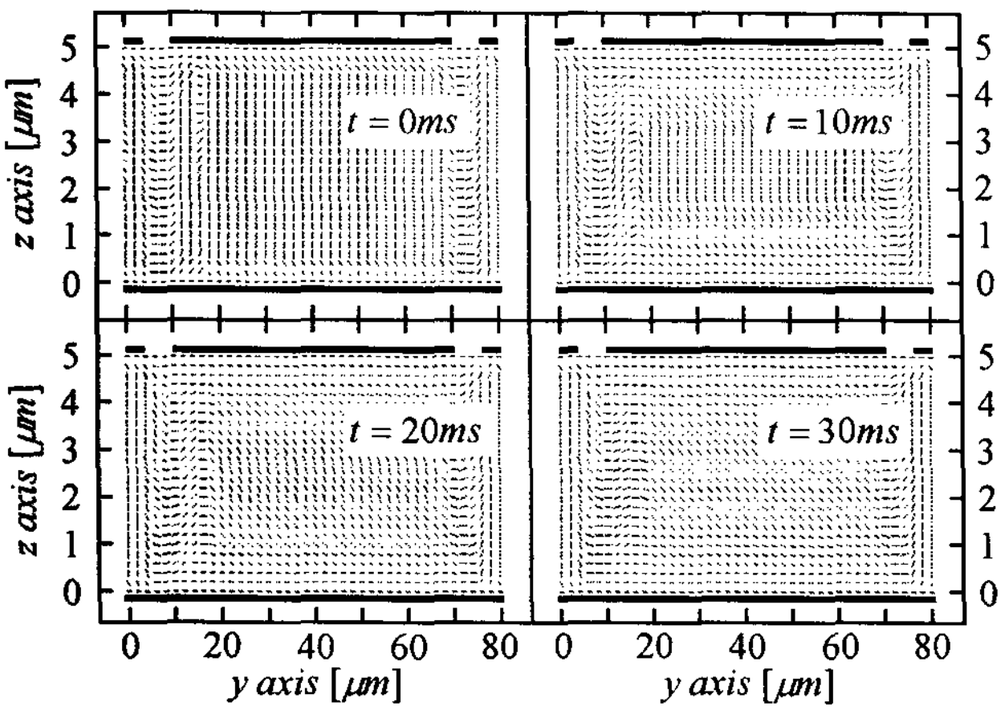
However, in the vector approach, since the disclination line is considered to the discontinuity of the director vector field, directors at the disclination line are going to lying for the first time to make the director field to a continuous profile. There are two reason to show such behaviors in the physical and mathematical meaning. First of all, very large distorsion energy is concentrated at the disclination line, thereby, the directors proceed in a way to reduce such a distortion energy. Moreover, the modeling equation of the vectorial form is simmilar to the form of diffusion equation which produce smooth profile from an discontinuous configuration.

On the other hand, in the tensor approach, once the disclination lines are formed by the electrical energy, the deformation is hardly found at that position because of the rod-like modeling of director, leading to nematic symmetry, that is, the equivalence of $\vec{n}$ and $-\vec{n}$. Therefore, the directors around the disclination line keep their direction aligning parallel to each other. Instead, by the surface strong anchoring and elastic torques between the neighboring directors, the relaxation of the normal and reverse tilt domain start and propagate toward the disclinaiton line. By the

conjunction of these two domain at that position, the disclination line is disappeared.



(a)tensor approach



(a) vector approach

Figure 1. The behaviors of director deformation profile for the vector and tensor approach. The relaxation of disclination line is found under the left side of pixel electrode. In the vector approach, the directors at the disclination line rotates first, while the directors at that position are aligned parallel to the neighboring directors in the tensor approach.

4. Conclusions

In this paper, we investigated dynamic behaviors of liquid crystal director profiles by simulating two different modeling equations based on vectorial and tensorial approaches. By performing 3-dimensional simulation for a unit pixel, we found that the simulation results from the each of modeling equations lead to different motional behaviors of liquid crystal directors around the disclination line. We used finite difference method as a numerical technique.

From the simulation results, it is clarified that the vectorial approach gives a way unlikely to happen, while the tensorial approach gives more realistic behaviors for the rotation of the directors around the disclination line. It is because the tensorial approach maintains nematic symmetry, that is, the equivalence of director $\vec{n}$ and its apposite $-\vec{n}$.

5. References

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