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Optical Simulation of Viewing Angle Property of Biaxial Nematic Bent-Core Liquid Crystal

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The conventional liquid crystal displays (LCDs) have been using optically uniaxial liquid crystal (LC) medium and this often causes a significant image change at oblique viewing angles. We simulated the viewing angle properties of the biaxial nematic (N_b) phase of a bent-core liquid crystal (BLC) and compared the results with the vertically aligned (VA)- and the in-plane switching (IPS)-LCDs. The N_b phase of the BLC showed a smaller transmittance at the dark state as well as a greater contrast ratio at wide viewing angle. The viewing angle property of the N_b-mode without any compensation film was slightly superior to the IPS-mode with the compensation films eliminating the decross of the polarizers at oblique viewing angle.

Keywords : Biaxial nematic liquid crystal, Viewing angle, Contrast ratio
OCIS codes : (160.3710) Liquid crystals; (120.2040) Displays; (160.1190) Anisotropic optical materials

I. INTRODUCTION

The bent-core liquid crystal (BLC) has been actively studied for last decades. The BLC medium showed various new physical properties and suggested important clues for understanding the underlying physics in the condensed matter [1-4]. The BLC also has a great potential of new electro-optical applications [5-13]. For example, some BLC molecules were found to have a larger flexoelectric effect than the conventional rodlike liquid crystal (LC) molecules [5-9]. Some BLC molecules were reported to have a strong nonlinear optical effect [10-13].

Among the various electrooptical properties of the BLC materials, the biaxiality of BLC in the nematic phase has probably drawn the most attention [14-18]. The conventional cylindrical LC materials used in liquid crystal display (LCD) are optically uniaxial (Fig. 1(a)). On the other hand, the BLC molecules have a biaxial shape and some of them were reported to have a biaxial ordering. Thus, the biaxial nematic phase (N_b) of BLC has three principal refractive indices possessing separate ordering of the long molecular axis as well as the short molecular axis (Fig. 1(b)). One of the merits of the N_b phase of BLC is the fast phase modulation of light by a rotation of the short molecular axes with their long molecular axes fixed. Because the friction of the molecules can be small, the short molecular axes switching process can be faster than the long molecular axes switching of the uniaxial nematic (N_u) phase materials [17, 18].

Meanwhile, the N_b material has a potential of a wider viewing angle than the N_u materials [19]. The phase retardation Γ of a uniaxial positive c-plate, which is equivalent to the vertically-aligned LCD (VA-LCD) at zero field state, for the light propagating along a polar angle θ and an azimuthal angle φ is given by,

$$\Gamma = \frac{2\pi}{\lambda}(n_e - n_o)d(\frac{n_e+n_o}{2n_o n_e^2})sin^2\theta \quad (1)$$

Here, n_e and n_o are the extraordinary and the ordinary refractive indices of the positive c-plate, respectively. Thus, Γ is significantly dependent on θ and this viewing angle dependence cannot be eliminated unless an additional negative c-plate is attached. Γ of a uniaxial positive a-plate, which is

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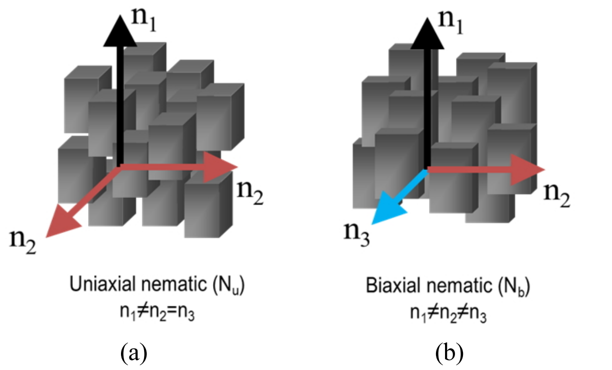

FIG. 1. Schematic illustration of the molecular orientation in (a) uniaxial nematic (N_u) and (b) biaxial nematic (N_b) phase.

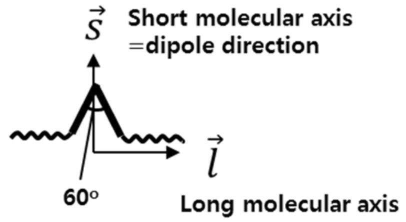

FIG. 2. The definition of the long molecular and short molecular axes of BLC. The LC orientation is determined by the long molecular axis ($\vec{l}$), while the dipole direction is parallel to the short molecular axis ($\vec{s}$).

equivalent to the zero field state of the in-plane switching (IPS)-LCD is given by,

$$\Gamma = \frac{2\pi}{\lambda}(n_e - n_o)d[1 + \frac{\sin^2\theta}{2n_o}\left(\frac{\sin^2\varphi}{n_e} - \frac{\cos^2\varphi}{n_o}\right)] \quad (2)$$

which also has some dependence on θ and φ. On the other hand, the phase retardation Γ of a biaxial retarder for the light propagating along θ and φ is given by,

$$\Gamma = \frac{2\pi}{\lambda}[(n_x - n_y) + (n_z^2 - n_x n_y)(\frac{\cos^2\phi}{n_y} - \frac{\sin^2\phi}{n_x})\frac{\sin^2\theta}{2n_z^2}]d \quad (3)$$

where, n_x, n_y, and n_z are the refractive indices of the material. Here, one of the principle axes was assumed to be aligned to the surface normal direction. The higher order terms were neglected. It is found that the dependence of Γ on θ and φ can be eliminated in Eq. (3) provided,

$$n_z^2 = n_x n_y \quad (4)$$

To our knowledge, there has been no detailed comparison of the viewing angle property of the N_b-LCD mode with the conventional VA- and IPS-LCD. We simulated the viewing angle dependence of the N_b-mode formed by the BLC molecules. We compared the viewing angle property of the N_b-mode with that of the VA- and IPS-modes. The N_b-mode showed a smaller transmittance (TR) at dark state and a greater contrast ratio (CR) at bright state than the VA- and IPS-modes.

II. METHODS

We considered a highly kinked BLC molecule with an apex angle ~60° (Fig. 2). The long molecular axis ($\vec{l}$) corresponds to the bow direction of the molecule. In our previous x-ray study [13], the alkyl chains of the highly kinked BLC were found to be parallel to $\vec{l}$. The long molecular axis $\vec{l}$ was aligned to the surface normal direction when the surface was coated with vertical alignment polyimide. The short molecular axis ($\vec{s}$) corresponds to the arrow direction of the molecule. Due to the narrow apex angle, the refractive index along $\vec{s}$ is greater than the one along $\vec{l}$. In addition, the dipole of the BLC is also parallel to $\vec{s}$ (Fig. 2). Thus, the BLC has a negative optical anisotropy Δn as well as a negative dielectric anisotropy $\Delta\varepsilon$.

The optical simulation was performed using the Extended Jones Matrix method [19] with a commercial LCD simulator Techwiz 2D (Sanayi system). The TR and CR values were calculated vs. θ and φ for a light of $\lambda = 550$ nm. The refractive indices of the LC layers used for the N_b-LCD were $n_x = 1.70$, $n_y = 1.50$, and $n_z = 1.60$ satisfying Eq. (4). We referred to the general refractive indices n_x and n_y in the previous literatures for the N_b-LCD simulation [20, 21]. The refractive indices of the VA- and the IPS-LCD were set to be $n_e = 1.70$ and $n_z = 1.50$. Thus, the average refractive indices and the maximum optical birefringence of the LC medium used for three modes were set to be the same in the simulations.

III. RESULTS AND DISCUSSION

For the N_b simulation, we considered the vertical orientation of the BLC molecules wherein $\vec{l}$ is aligned to the surface normal direction (z-axis) (Fig. 3(a)). $\vec{s}$ is aligned to the x-axis and the sample has D_{2h} symmetry. The orientation of $\vec{s}$ is determined by unidirectional rubbing of the surface in the experiments. The transmission axis of the polarizer and the analyzer was at 0° and 90° to the x-axis. Thus, the BLC sample in the N_b phase has no TR at zero field state, i.e., normally black mode. At bright state, $\vec{s}$ is switched to 45° to the transmission axis of the polarizer and this can be induced by applying an in-plane electric field in the experiments. The LC directors in the VA-LCD was vertically aligned at zero field state and switched to planar state with the optic axis oriented 45° to the polarizer (Fig. 3(b)). The LC directors in the IPS-LCD was planar aligned at zero field state parallel to the polarizer and switched to 45° to

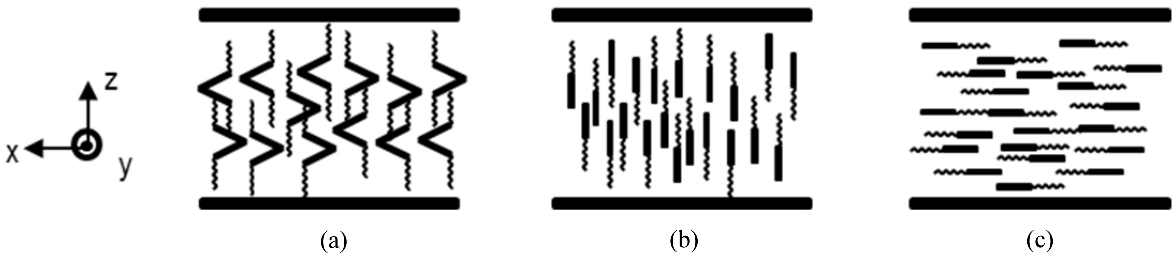

FIG. 3. The orientation of the LC molecules in (a) N_b-, (b) VA-, and (c) IPS-modes at dark state. The transmission axis of the polarizer is along *x*-axis.

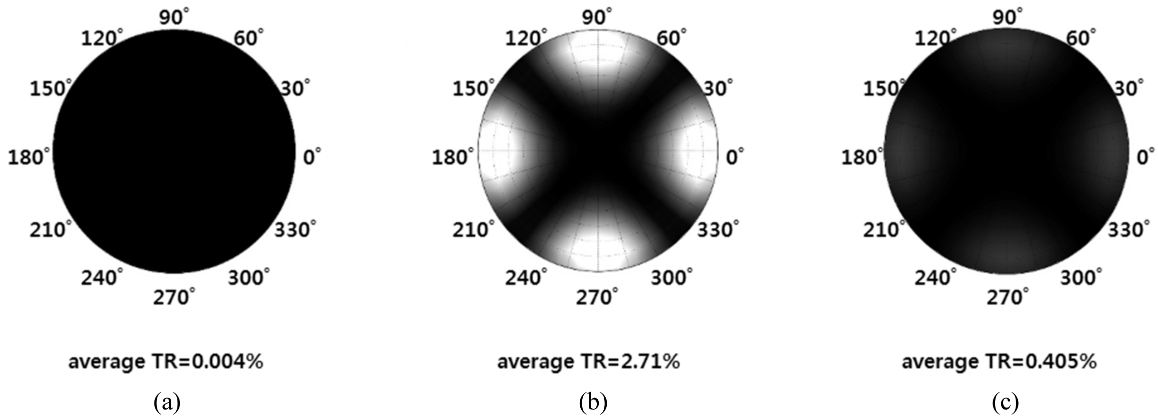

FIG. 4. Simulation results of TR of (a) N_b-, (b) VA-, and (c) IPS-modes at dark state.

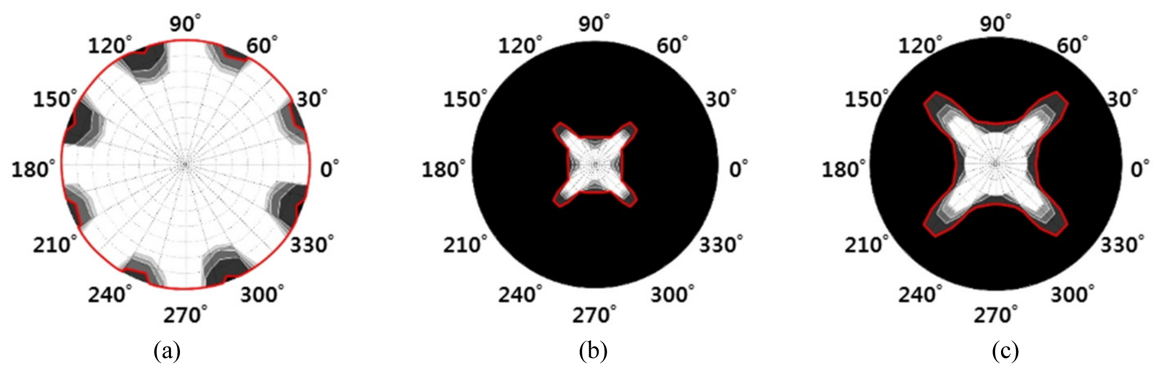

FIG. 5. Simulation results of CR of (a) N_b-, (b) VA-, and (c) IPS-modes. Red line in the figure corresponds to the viewing angle with CR=800:1.

the polarizer (Fig. 3(c)).

Figure 4 shows the optical simulation results of TR of the N_b-, VA-, and IPS-modes at dark state. The contour scales were the same through Fig. 4(a)-(c). It is clearly observed that the N_b-mode shows uniform dark state through the whole viewing angle (Fig. 4(a)). The average TR of the N_b-mode was 0.004%. The least viewing angle dependence of the N_b-mode is due to the elimination of θ and φ terms in Eq. (3) by substituting LC refractive indices satisfying Eq. (4). On the other hand, the VA-mode showed a significant light leakage at wide polar viewing angle (Fig. 4(b)). This is due to the increase of Γ with increasing θ in Eq. (1). The average TR of the VA-mode was 2.71%. The IPS-mode showed an intermediate viewing angle dependence of TR. The smaller light leakage of the IPS-mode than the VA-mode is due to the smaller dependence of Γ on θ and φ in Eq. (2). The average TR of the IPS-mode was 0.405%.

Figure 5 shows the simulation results of CR of the N_b-, VA-, and IPS-modes with the same scales. For the calculation of CR, we assumed uniform orientation of LC directors at bright state. The red line in each figure corresponds to the viewing angle with CR=800:1. The N_b-mode showed CR > 800:1 when θ >80^o regardless of φ. On the other hand, the VA- and the IPS-mode showed CR=800:1 when θ =20^o

and 30^o regardless of φ, respectively. Thus, it is clearly observed that the N_b-mode shows much wider viewing angle property of CR than the VA-, and the IPS-modes. The wider viewing angle keeping the high CR value is mainly due to the small TR at the dark state in Fig. 4(a).

We also compared the CR value of the N_b-, the VA-, and the IPS-modes with compensation films attached (Fig. 6]. The compensation film of the N_b-LCD is composed of a pair of a positive a- and a negative a-plate whose optic axes are orthogonally oriented (Fig. 6(a)). These retarders compensate the decrossing of the absorption axes of the polarizer and the analyzer at oblique viewing angle [19]. The viewing angle dependence of CR of the N_b-LCD was slightly improved after attaching the compensation film, but the change was not very large. The compensation film of the VA-mode is composed of a negative c-plate with a retardation of $-\lambda/2+\lambda/2\pi$ and a positive a-plate with a retardation of $\lambda/4$ (Fig. 6(b)). This combination of retarder compensates the change of Γ by the LC as well as the decrossing of the polarizers at oblique viewing angle [19]. The viewing angle property of the VA-modes was much improved after attaching the compensation film. Although the retarder films used for the VA-mode compensated the change of Γ by the LC as well as the decrossing of the polarizers at oblique viewing angle, the viewing angle property of the VA-mode was inferior to that of the N_b- and IPS-mode. The compensation film used for the IPS-LCD simulation was the same as the one used in the N_b-mode (Fig. 6(c)). The viewing angle property of the IPS-mode was also much improved after attaching the compensation film. Nevertheless, the viewing angle dependence of CR of the N_b-mode was still superior to the IPS-mode. Moreover, the viewing angle of the N_b-mode without the compensation film (Fig. 5(a)) was still better than that of the IPS-mode with the compensation film (Fig. 6(c)).

Although there have been many efforts to develop the N_b-material which operates at room temperature, few materials with a wide nematic phase around room temperature has been reported [22]. With this reason, the electrooptical properties of the BLC molecules for the display applications have been focused in the smectic or isotropic phases [23-25]. For the practical application of N_b-mode LCD, new BLC materials possessing a wide nematic phase range around room temperature should be synthesized [20]. Alternatively, mixing the BLC molecules with the conventional rodlike LC can be another solution [6-9]. Although the miscibility between the molecules are not very good due to their different shapes and molecular weights, a small amount of BLC less than 10 wt% can contribute to the improvement of the viewing angle, provided the mixtures possess biaxial ordering. In addition, a robust alignment technique to align the long molecular axes as well as the short molecular

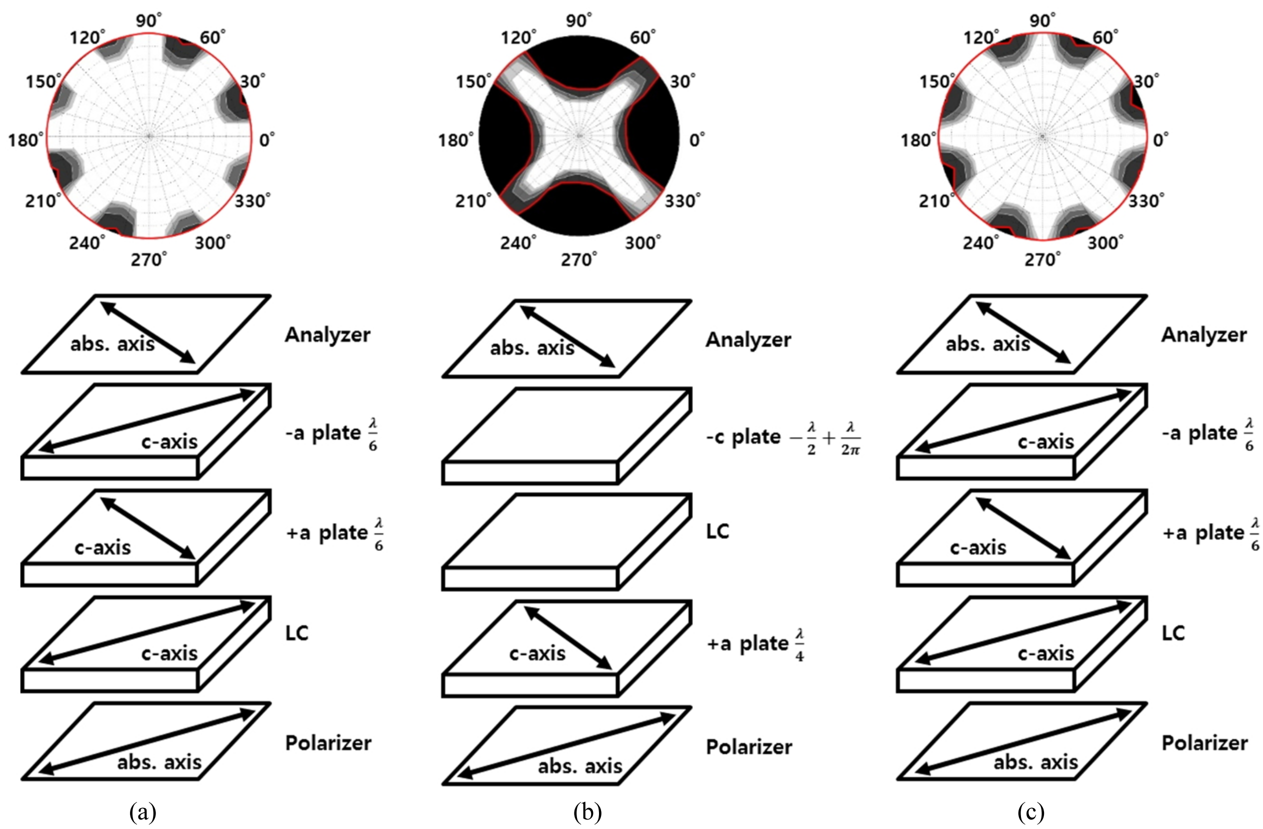

FIG. 6. Simulation results of CR of (a) N_b-, (b) VA-, and (c) IPS-modes with compensation films. The structures of the compensation films are shown in the schematic drawing.

axes, i.e., inducing the biaxial ordering, should be developed. Although an experimental realization and a commercial application of the N_b-phase still requires more time, the suggested optical simulation study confirms its superior performance as future phase modulation components.

IV. CONCLUSION

To summarize, we simulated the viewing angle properties of the N_b-mode made from BLC molecules, and compared the results with the ones of the VA- and IPS-modes. The N_b-mode showed a smaller TR at dark state as well as a greater CR at wide viewing angle. The viewing angle property of the N_b-mode without any compensation film was slightly superior to the IPS-mode with compensation films eliminating the decrossing effect of the polarizers at oblique viewing angle.

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