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The Novel 8x8 Transfer Matrix Method of the LC Optics Simulations: Application to Reflective LCDs

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A new effective matrix method for the calculation of optical characteristics of Reflective Liquid Crystal Displays (RLCDs) with consideration for multiple reflection is proposed.

Keywords: optical simulation; LCD optimization; reflection

INTRODUCTION

The accurate calculation of reflectance in a variety of Reflective Liquid Crystal Displays (RLCDs), in particular, in one-polarizer constructions of RTN- and RSTN-RLCDs^[1], has to provide a corresponding allowance for the whole construction of the LCD, including the optical contribution of the thin current-conducting and aligning layers. The optics of the multi-layer LCD structure should involve multiple reflections. The method of complex 4x4 matrices (C4x4MM) can be used for the purpose^[2-6]. One of the drawbacks of this method is a necessary spectral averaging, which is time-consuming^[7]. The paper shows, that the transfer 8x8 matrix method, developed by one of the authors^[8] remains the most effective in this case. This method provides the same accuracy, as complex 4x4

matrices technique with a spectral averaging, but is 50-70 times faster. Recently we successfully applied the method for the optimization of the contrast ratio of the Reflective LCDs with AR layers in LCD construction^[9].

THEORY

When the spectral averaging in the C4×4MM method is used to model the LCD transmittance and reflectance we have to take into account the real measurements conditions, i.e. the application of a non-coherent broadband light source and monochromator, transmitting the quasi-monochromatic light with a relatively large spectral bandwidth $\Delta\lambda$. Usually $\Delta\lambda$ is equal to 4-10 nm. The C4×4MM method deals with the calculations of the transmittance and reflectance of the layered structures in a monochromatic (coherent) light. Allowing for the measurements conditions we have to make the convolution of the obtained by C4×4MM method coherent LCD spectra with a spectral window $\Delta\lambda$, i.e. spectral averaging. Common procedure of the spectral averaging is considerably time-consuming due to the presence of the fast oscillations on the model coherent LCD spectra, caused by Fabry-Perot (FPI) interference in relatively thick layers (glass substrates, polarizers etc.) Generally the interval $\Delta\lambda$ contains dozens of FPI interference peaks. Transfer 8x8 matrix method, based on the theory of partial coherence^[10] and the C4×4MM method theory, allows to obtain the transmittance and reflectance of stratified media directly for the incident quasi-monochromatic light without the spectral averaging and is only 20%-50% more time consuming, than C4×4MM method, when calculating the coherent transmittance and reflectance. Transfer 8x8 matrix method is applied to simulate the LCD optics in terms of the propagation of the plane quasi-monochromatic wave in a special one-dimensional non-uniform layered structure that models the LCD configuration.

FPI effect in a quasi-monochromatic light in a layer of a thickness d is known to take place dependent on the relationship between the

coherence length l_{coh} of the incident light and the value of d . The multibeam interference (FPI) takes place when $d \ll l_{coh}$. In this case the visibility of fringes remains almost the same, as for a monochromatic light. Those layers and layer systems we will denote as «thin-layer» elements. If $d > l_{coh}$ the multiple-reflected waves will not interfere and the total intensity will be the sum of the intensities of the constituent waves. Those layers are denoted as «thick» elements. At the intermediate d values a smoothed interference pattern will be observed. The common measured transmittance and reflectance LCD spectra correspond to the incident light with a coherence length of 30-150 μm ($l_{coh} \sim \tilde{\lambda}^2 / \Delta\lambda$, where $\tilde{\lambda}$ - the averaged wavelength^[10]). If we select $l_{coh} \approx 100 \mu\text{m}$, we may divide the LCD construction to the «thick» and «thin» elements. The «thick» elements are the glass substrates ($d \sim 1 \text{ mm}$), polarizers ($d \sim 200 \mu\text{m}$) etc. The «thin» elements are usually include the LC layer ($d < 10 \mu\text{m}$), current-conducting and aligning layer structures ($d < 1 \mu\text{m}$), anti-reflective (AR)-films ($d < 1 \mu\text{m}$) etc.

The layered “thin” and “thick” elements structure can be divided into the fragments, which approximately obey the following rules (Fig.1):

- (i) all the waves generated within the fragment by the incident on the fragment wave W_1 (or W_2) are summed as coherent waves;
- (ii) all the waves generated by W_1 are summed with the wave generated by W_2 as non-coherent waves.

These substructures we will define as D-fragments. The following D-fragments can be distinguished in the layered system:

1. The boundary between “thick” layers.
2. “Thin-layer” element located between the “thick” layers.
3. The bulk of “thick” layer (the “thick” layer without its boundary).
4. The boundary between the “thick” layers plus the bulk of one or both of the contacting “thick” layers.
5. “Thin-layer” system located between the “thick” layers plus the bulk of one or both of the neighbor “thick” layers.

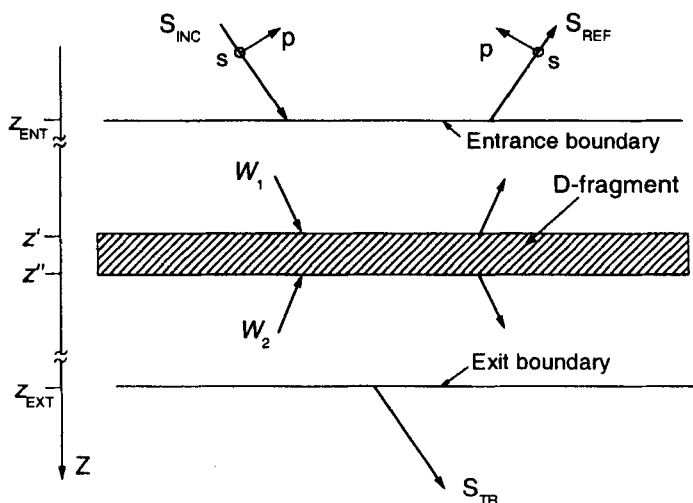


FIGURE 1. To the definition of D-fragment. Geometry of the problem.

Figure 2. (variant A) shows a possible separation of one-polarizer RLCD into the D-fragments by comparing the incident light coherence length and the thickness of the LCD constituent layers. After dividing the layered structure into D-fragments we may use transfer 8×8 matrix formalism^[8] to describe the spatial evolution of characteristics of the light propagated in LCD.

Consider some layered structure, located in the region $z_{\text{ENT}} \leq z \leq z_{\text{EXT}}$ (axis z of the Cartesian coordinate system xyz goes parallel to the direction of stratification), and let the plane quasi-monochromatic wave is incident from the space $z < z_{\text{ENT}}$ (Fig.1). Let the structure can be divided into D-fragments. Represent the total electric field \mathbf{E} induced in the layered structure by the incident wave in the form of the expansion in natural-wave basis^[4-6,8].

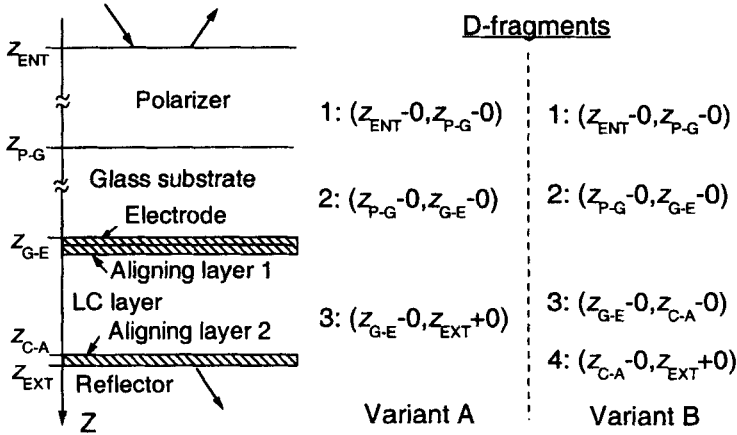


FIGURE 2. D-fragments in one-polarizer RLCD. Variant A: FPI in LC layer is allowed for; variant B: the pattern of FPI in LC layer is eliminated.

$$\mathbf{E}(z, t) = \sum_{j=1}^4 \mathbf{e}_j(z) A_j(z, t),$$

where \mathbf{e}_j is the oscillation vector of electric field of j -th basis natural wave^[6], A_j ($j=1,2,3,4$) are the scalar complex amplitudes of the natural-wave components of the total field. The amplitudes A_j are random functions of time. Consider the basis waves with $j=1,2$ propagating in $+z$ -direction, while the waves with $j=3,4$ - in $-z$ -direction. We will take the real correlation 4-columns, as the statistical characteristics of the wave fields, propagating in $+z$ and $-z$ directions:

$$\bar{\mathbf{S}}(\mathbf{r}) = \mathbf{L} \langle \bar{\mathbf{a}}(\mathbf{r}, t) \otimes \bar{\mathbf{a}}(\mathbf{r}, t)^* \rangle \quad (+z\text{-direction})$$

and

$$\bar{\mathbf{S}}(\mathbf{r}) = \mathbf{L} \langle \bar{\mathbf{a}}(\mathbf{r}, t) \otimes \bar{\mathbf{a}}(\mathbf{r}, t)^* \rangle \quad (-z\text{-direction}),$$

where

$$\mathbf{L} = \begin{pmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & -i & i & 0 \end{pmatrix}, \bar{\mathbf{a}}(\mathbf{z}, t) = \begin{pmatrix} \mathcal{A}_1(\mathbf{z}, t) \\ \mathcal{A}_2(\mathbf{z}, t) \end{pmatrix}, \bar{\mathbf{a}}(\mathbf{z}, t) = \begin{pmatrix} \mathcal{A}_3(\mathbf{z}, t) \\ \mathcal{A}_4(\mathbf{z}, t) \end{pmatrix},$$

\otimes denotes the Kronecker matrix product^[11], $\langle \rangle$ means the time averaging. Let us point out, that the columns $\bar{\mathbf{S}}$ and $\bar{\mathbf{S}}$ are very similar to Stokes vectors^[12]. The Ref. [8] states, that the correlation columns near the boundaries of each D-fragment can be related as follows:

$$\begin{aligned} \bar{\mathbf{S}}(z'') &= \tilde{\mathbf{D}}(z'', z') \bar{\mathbf{S}}(z'), \\ \bar{\mathbf{S}}(z) &\equiv \begin{pmatrix} \bar{\mathbf{S}}(z) \\ \bar{\mathbf{S}}(z) \end{pmatrix}, \quad \tilde{\mathbf{D}}(z'', z') = \mathbf{D}\{\mathbf{T}(z'', z'; \tilde{\lambda})\}. \end{aligned} \quad (1)$$

Here z' and z'' are the z -coordinates of D-fragment boundaries; $\mathbf{T}(z'', z'; \lambda)$ is the complex 4x4 transfer matrix, that connects 4-columns of the complex amplitudes $\mathbf{A} = (A_1, A_2, A_3, A_4)^T$ near the boundaries of the fragment, i.e. $\mathbf{A}(z'') = \mathbf{T}(z'', z'; \lambda) \mathbf{A}(z')$, when the monochromatic light with the wavelength λ is incident on the structure; $\tilde{\lambda}$ is the average wavelength of the incident quasi-monochromatic light; $\tilde{\mathbf{D}}\{\mathbf{T}\}$ is the real 8x8 matrix calculated from 4x4 matrix \mathbf{T} as follows:

$$\tilde{\mathbf{D}}\{\mathbf{T}\} = \begin{pmatrix} \mathbf{L}[\mathbf{t}_{11} \otimes (\mathbf{t}_{11} - \mathbf{t}_1) - \mathbf{t}_1 \otimes \mathbf{t}_{11}] \tilde{\mathbf{L}} & \mathbf{L}(\mathbf{t}_{12} \otimes \mathbf{t}_{12}) \tilde{\mathbf{L}} \\ -\mathbf{L}(\mathbf{t}_{21} \otimes \mathbf{t}_{21}) \tilde{\mathbf{L}} & \mathbf{L}(\mathbf{t}_{22} \otimes \mathbf{t}_{22}) \tilde{\mathbf{L}} \end{pmatrix}, \quad \mathbf{t}_1 = \mathbf{t}_{12} \mathbf{t}_{22}^{-1} \mathbf{t}_{21},$$

$$\tilde{\mathbf{L}} = \mathbf{L}^{-1};$$

\mathbf{t}_{ij} are the 2x2 matrix blocks of $\mathbf{T} \equiv \begin{pmatrix} \mathbf{t}_{11} & \mathbf{t}_{12} \\ \mathbf{t}_{21} & \mathbf{t}_{22} \end{pmatrix}$. The matrix $\mathbf{T}(z'', z'; \lambda)$

can be easily calculated using C4x4MM method. We denote $\tilde{\mathbf{D}}(z'', z')$ matrix as a transfer 8x8 matrix of the fragment (z'', z') . The layered structure as a whole is described by transfer 8x8 matrix $\mathbf{D}_s \equiv \mathbf{D}(z_{\text{EXT}} + 0, z_{\text{ENT}} - 0)$, that couples the columns $\bar{\mathbf{S}}(z_{\text{ENT}} - 0)$ and

$\bar{\mathbf{S}}(z_{\text{EXT}} + 0)$, characterizing the light field near the external boundaries of the structure (Fig.1):

$$\bar{\mathbf{S}}(z_{\text{EXT}} + 0) = \mathbf{D}_s \bar{\mathbf{S}}(z_{\text{ENT}} - 0). \quad (2)$$

In accordance with (1) we may calculate the matrix \mathbf{D}_s as a product of the transfer 8x8 matrices of the constituent D-fragments. In the above example (Fig.2, variant A) \mathbf{D}_s is calculated according to the formula:

$$\mathbf{D}_s = \mathbf{D}(z_{\text{EXT}} + 0, z_{\text{G-E}} - 0) \mathbf{D}(z_{\text{G-E}} - 0, z_{\text{P-G}} - 0) \mathbf{D}(z_{\text{P-G}} - 0, z_{\text{ENT}} - 0).$$

Here z_{ENT} , $z_{\text{P-G}}$, $z_{\text{G-E}}$, z_{EXT} are z-coordinates of the air-polarizer, polarizer-substrate, substrate-electrode, aligning layer 2-reflector boundaries, respectively. Taking into account the boundary conditions we may easily calculate from \mathbf{D}_s matrix the transmittance and reflectance of the layered structure. Thus the reflectance matrix $\bar{\mathbf{R}}_s$ of the layered structure, that couples the correlation columns of the incident (\mathbf{S}_{INC}) and reflected light (\mathbf{S}_{REF}) (Fig.1) $\mathbf{S}_{\text{REF}} = \bar{\mathbf{R}}_s \mathbf{S}_{\text{INC}}$ can be found as

$$\bar{\mathbf{R}}_s = -\mathbf{d}_{22}^{-1} \mathbf{d}_{21},$$

where \mathbf{d}_{ij} are the 4x4-blocks of matrix $\mathbf{D}_s \equiv \begin{pmatrix} \mathbf{d}_{11} & \mathbf{d}_{12} \\ \mathbf{d}_{21} & \mathbf{d}_{22} \end{pmatrix}$. If in the example (Fig.2) we take the basis natural waves with $j=1,3$ as p-polarized, and ones with $j=2,4$ as s-polarized (Fig.1) and normalize the vectors \mathbf{e}_j in accordance with the condition $\mathbf{e}_j \mathbf{e}_j = 1$, then the matrix $\bar{\mathbf{R}}_s$ will be Mueller reflectance RLCD matrix in the basis of p- and s-polarizations^[12]. The {1,1} element of this matrix should be equal to value of the RLCD reflectance for a non-polarized light.

SIMULATION RESULTS

Figure 3 presents the reflectance spectra for RTN-mode RLCD^[11], calculated for the following typical parameters of the device elements.

1. LC layer : $K_{11}=1.3 \cdot 10^{-6}$ dyne, $K_{33}/K_{11}=1.5$,
 $K_{22}/K_{11}=0.546$, $\epsilon_{\parallel}=15.1$, $\epsilon_{\perp}=3.8$, $d=5.3\mu\text{m}$,

- $n_{||}(437\text{nm}) = 1.649$, $n_{\perp}(437\text{nm}) = 1.538$,
 $n_{||}(546\text{nm}) = 1.623$, $n_{\perp}(546\text{nm}) = 1.523$,
 $n_{||}(644\text{nm}) = 1.612$, $n_{\perp}(546\text{nm}) = 1.517$,
 twist angle = 52° , pretilt angle = 2° ;
 2. Glass substrate: $n=1.52$, $d=1\text{mm}$.
 3. Current-conducting layer: $n=2.05$, $d=0.03\mu\text{m}$.
 4. Aligning layer: $n=1.6$, $d=0.1\mu\text{m}$.
 5. Polarizer: $d=200\mu\text{m}$, $n_{\perp}=1.52+i\times 2.23\times 10^{-5}$, $n_{||}=1.5201+i\times 1.5\times 10^{-3}$, the transmission axis is parallel to the rubbing direction on the entrance substrate.
 6. Reflector: $n=0.2+i\times 3.44$.
 7. RLCD: $U_{\text{off}} = 0\text{ V}$, $U_{\text{on}} = 2.25\text{V}$, normal light incidence.

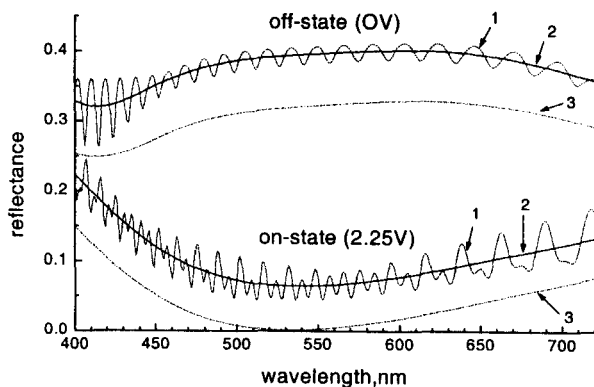


FIGURE 3. Simulation of RLCD spectra using D-matrix approach: 1- FPI effect in LC layer; 2 - smoothed spectra, the pattern of FPI in LC layer is eliminated; 3 - spectra calculated without considering the parasitic reflections, reflection from the reflector only is allowed for.

Figure 3 shows, that the high frequency oscillations, caused by FPI effect in thick layers, which are common for the model coherent spectra are absent, when the non-coherent wave approach applies. The curves 1 in Figure 3 correspond to the spectra of RLCD calculated by

D-fragment separation in accordance with the variant A (Fig.2). The LC layer was treated as a "thin" element and the FPI effect give the corresponding oscillations of reflectance. This can really take place in case of a perfect uniformity of the LC layer thickness over the surface area. However, it is more convenient to neglect FPI into LC layer during the optimization procedure and to analyze the smoothed spectra. To eliminate the FPI pattern into LC layer from the simulated spectra, we have to consider the LC layer as a "thick" element in the process of the D-fragments separation. The variant B (Fig.2) directly corresponds to the case. In the case the matrix D_s can be calculated as:

$$D_s = D(z_{EXT} + 0, z_{C-A} - 0) D(z_{C-A} - 0, z_{G-E} - 0) D(z_{G-E} - 0, z_{P-G} - 0) D(z_{P-G} - 0, z_{ENT} - 0),$$

where z_{C-A} is z-coordinate of LC-aligning layer 2 boundary.

The corresponding smoothed spectra are shown in Fig.2 as solid lines. The smoothed spectra can be obtained much faster, than the FPI spectra related to the variant A in Fig.2. To underline the importance of the glare reflections in RLCD spectra, we showed in Fig.3 the reflectance spectra, that does not allowed for the reflections from the outer RLCD surface as well as from the conducting and aligning layers of RLCD.

CONCLUSION

The new method of the simulation of RLCD reflectance taking into account the glare reflections is proposed. The method has the same accuracy, but is more fast and efficient, than the method of spectral averaging in 4x4 matrix approach.

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