Characterization of inhomogeneous retarders

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Abstract
This paper presents various approaches for measurement and evaluation of optical characteristics of compound retarder sheets and discusses their features and limitations. We introduce and compare two ways of modeling the actual multilayer structure with an inclined uniaxial indicatrix and an inhomogeneous biaxial layer plus negative c-plate, and the performance of these models is analyzed for the principle plane of light incidence and for arbitrary directions of light propagation.

1. Introduction
Detailed analysis of liquid crystal display devices (LCDs) via numerical modeling has become indispensable in the research and development of new electro-optical effects in LCs and for the optimization of existing LC-display effects because it allows exact and individual control of all parameters of the implemented model and it provides fast results, thus being an ideal complement to the laboratory workbench [1].

In state-of-the-art LCDs two approaches are used for reducing the variation of luminance, contrast and chromaticity with viewing-direction, i.e. for "widening" the viewing-cone:

- LC-alignment in multi-domain configurations induced by surface treatment or structures or by the electric field and
- application of birefringent retarder sheets.

Accurate numerical modeling and detailed optimization of the LC-display system requires precise knowledge of the physical parameters of the relevant materials and components including polarizers and retarders. These target parameters are the thickness of the layers, their complex refractive indices (in order to account for absorption) vs. wavelength of light and the spatial distribution of the optical axes. Unfortunately, the parameters that are usually available from manufacturers or published in the literature are not the ones required for the detailed numerical model. Instead they are too generic (e.g. birefringence and retardation of layer) and thus far from being sufficient, precise and complete.

Methods for characterization of retarders include ellipsometry [4, 5], fitting of measured retardation versus angle of inclination in the plane of symmetry [6, 7, 8], numerical fitting of the transmittance of polarized light as a function of the direction of propagation [9], and finally, numerical fitting of the directional distribution of generalized anisotropic ellipsometry data to obtain the refractive indices together with the director field across the layer [10].

Figure 1: Improvement of the viewing-cone the TN-effect with two generations of retarder sheets (figures from Mori. et. al. [2]).

Figure 2: Viewing-cone of retarder-sheet compensated TN-LCDs in various state-of-the-art commercial computer monitors [3].

Figure 3: Typical 1D layer-structure of an LCD with polarizers, retarders, electrodes and other layers and components in DIMOS.
In a series of papers, Yamahara [6] has published a method of fitting the measured retardation vs. angle of inclination (within the symmetry plane of the discotic layer) to the simple model of a homogeneously inclined biaxial indicatrix. As a result of these evaluations the local refractive indices are obtained together with the angle of inclination of the biaxial indicatrix, $\theta$, from which a global anisotropy value, $R_{th}$, is calculated for characterization of the retarder. A variety of samples of the Fuji Wide-View film, comprising a TAC-layer and a splayed discotic layer [8], were measured by Yamahara and as a consequence of the results obtained with his method, the author approximates the global optical behaviour of the Wide-View film by a uniformly inclined uniaxial indicatrix.

Figure 4: Details of a typical 1D layer-structure of an LCD with polarizers, retarders, electrodes and other layers and components.

An even more simple model applied to the evaluation of the local indices of refraction of a retarder made from tilted discotic phases, as published by Wu [7], uses an average refractive index as an approximation for calculation of the direction of light propagation within the birefringent retarder. In severe cases the three unknown parameters for this simple model are not even obtained by fitting of many data points, but they are estimated from three individual retardation values measured at three angles of inclination.

Figure 5a: Layer of a compound retarder with varying inclination of the optical axis of the discotic material.

Figure 5b: Typical layer-structure of a retarder with two TAC-layers and one active PVA-iodine layer.

2. Experimental
The retardation of our retarder samples has been measured with a Woollam multiwavelength ellipsometer [11] at wavelengths of 450 nm, 550 nm and 610 nm over a range of inclination angles from -60° to +40° with steps of 1°. From the numerical fitting of the measured retardation values to two retarder models we obtain the local indices of refraction, $n_a$, $n_b$ and $n_c$ as listed in table 1.

2.1 Single-layer models
Approximating the compound retarder by a single birefringent layer with the quantities shown in figs. 6 and 7, the retardation, i.e. the optical path difference between the s and p-polarized beam is given by (compare e.g. Yeh and Gu, 12):

\[
\Gamma_i = n_{eff} (\theta_p) \cdot AB + BC - n_a \cdot AC
\]

with the effective index of refraction for the p-polarized beam, $n_{eff}$.
the angle of inclination of the p-polarized beam according to

and after some arithmetic manipulations, we obtain solutions for

The terms A, B and C are given by:

\[ A = (n_b^2 \sin^2 \alpha + n_c^2 \cos^2 \alpha) \]

\[ B = 2 \cdot \sin \alpha \cdot \cos \alpha \cdot (n_b^2 - n_c^2) \]

\[ C = (n_b^2 \cos^2 \alpha + n_c^2 \sin^2 \alpha) - \frac{n_b^2 \cdot n_c^2}{\sin^2 \theta} \]

With the continuity condition according to Snell

\[ \sin \theta = \sin \theta_p \cdot n_{\text{eff}}(\theta_p) = \sin \theta_s \cdot n_a \]

With the angular conventions used here, the sign of the root has to

The terms A, B and C are given by:

\[ A = (n_b^2 \sin^2 \alpha + n_c^2 \cos^2 \alpha) \]

\[ B = 2 \cdot \sin \alpha \cdot \cos \alpha \cdot (n_b^2 - n_c^2) \]

\[ C = (n_b^2 \cos^2 \alpha + n_c^2 \sin^2 \alpha) - \frac{n_b^2 \cdot n_c^2}{\sin^2 \theta} \]

This result is different from the result of Yamaha [6] where a

with an average index of refraction \( n^* \)

\[ \sin \theta = n^* \cdot \sin \theta^* = \frac{n_b + 2 \cdot n_c \cdot \sin \theta^*}{3} \]

equation (1) becomes

\[ \Gamma_i = n_{\text{eff}}(\theta_p) \cdot \Delta \mathbf{B} - n_a \cdot \Delta \mathbf{B} = -\frac{d}{\cos \theta^*} \left( n_{\text{eff}}(\theta_p) - n_a \right) \]

which is equivalent to the formula of Wu [5]:

\[ \Gamma = d_{\text{eff}} \cdot \Delta n_{\text{eff}} = \frac{d}{\cos \theta^*} \left( n_a \cdot n_c \cdot \sin^2 \alpha - \frac{n_b \cdot n_c}{\sin^2 \theta} \right) \]
2.4 Out-of-plane performance

In order to accurately evaluate the performance of the described model and the respective results we have used DIMOS [1, 14, 15] to compute the directional variation of transmittance for the single layer model and to compare it with measured results as shown in fig. 8. The model for the compound retarder in DIMOS comprises both a TAC-layer (uniaxial negative c-plate) and a splayed biaxial discotic layer with linear variation of the tilt angle of the local optical axis. It can be seen in fig. 9 that the biaxial single-layer model with constant tilt produces a directional transmittance distribution that is always symmetric with respect to the plane containing the b-axis of the indicatrix according to fig. 7 (here the vertical axis) while the measured directional distribution does not show this symmetry (compare [9]).

For the TAC-layer the following parameters are used to yield an out-of-plane retardation $R_{th} = -40nm$:

- $n_a = 1.480$, $n_b = 1.480$, $n_c = 1.396$ @ 0.1 mm thickness

By iterative adjustment of the refractive indices of the discotic layer (with linear tilt), starting from the values of Mori [8] at a fixed layer-thickness of 2 $\mu$m, we arrive at the following values:

- $n_a = 1.564$, $n_b = 1.578$, $n_c = 1.528$ with $\theta = 10^\circ - 65^\circ$

The results obtained for the local refractive indices $n_a$, $n_b$, and $n_c$, and retardations for the entire film $d\Delta n_{xz}$ and $d\Delta n_{zy}$, obtained by numerical fitting to the two single-layer models and different boundary conditions and constraints for $n_a$. Yellow field show the results of the free parameters obtained by the fitting, red values of $n_a$ were fixed during fitting.

Table 1:

<table>
<thead>
<tr>
<th>$n_a$</th>
<th>$n_b$</th>
<th>$n_c$</th>
<th>$\theta$</th>
<th>RMS-error</th>
<th>$d\Delta n_{xz}$</th>
<th>$d\Delta n_{zy}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>450 nm</td>
<td>1.483037</td>
<td>1.482873</td>
<td>1.481531</td>
<td>18.2</td>
<td>0.60601900</td>
<td>-110.1685</td>
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<td></td>
<td>1.600000</td>
<td>1.599830</td>
<td>1.598395</td>
<td>18.16</td>
<td>1.41799677</td>
<td>-117.9215 (7.0%)</td>
</tr>
<tr>
<td>Wu</td>
<td>1.481400</td>
<td>1.481237</td>
<td>1.479947</td>
<td>18.92</td>
<td>0.630522504</td>
<td>-117.7954 (6.9%)</td>
</tr>
<tr>
<td>550 nm</td>
<td>1.482803</td>
<td>1.482681</td>
<td>1.481376</td>
<td>16.14</td>
<td>0.53884205</td>
<td>-112.4960</td>
</tr>
<tr>
<td></td>
<td>1.600000</td>
<td>1.599871</td>
<td>1.598459</td>
<td>15.99</td>
<td>1.45678369</td>
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</tr>
<tr>
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<td>1.481279</td>
<td>1.480008</td>
<td>16.55</td>
<td>0.668474915</td>
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</tr>
<tr>
<td>610 nm</td>
<td>1.480286</td>
<td>1.481767</td>
<td>1.478872</td>
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<td>1.599883</td>
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</tr>
<tr>
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<td>1.481290</td>
<td>1.480028</td>
<td>15.61</td>
<td>0.507970822</td>
<td>-119.3609 (3.9%)</td>
</tr>
</tbody>
</table>

Table 1: Comparison of the results obtained for the local refractive indices $n_a$, $n_b$, and $n_c$, and retardations for the entire film $d\Delta n_{xz}$ and $d\Delta n_{zy}$, obtained by numerical fitting to the two single-layer models and different boundary conditions and constraints for $n_a$. Yellow field show the results of the free parameters obtained by the fitting, red values of $n_a$ were fixed during fitting.
3 Discussion

The results for the layer retardations $d\Delta n_{zx}$ and $d\Delta n_{zy}$ listed in table 1 together with the respective RMS-error, indicating the quality of the fit, illustrate that quite different solutions can be obtained depending on the fixed boundary conditions during the fitting procedure. We see that the more detailed model (used also by Yamahara [6]) does not necessarily provide better modeling of the compound retarder since the assumption of $n_a = 1.6$ as used here is too far from the actual value which is rather close to 1.48. This assumption is the cause for errors in the layer-retardations $d\Delta n_{zx}$ and $d\Delta n_{zy}$ which are often used for characterization of retarders of up to 9.9%.

Three solutions corresponding to 3 local minima in the range for $n_a$ from 1.48 to 1.60 can be compared to each other by the quality of their fitting (RMS-error) as a way to reduce the ambiguity of the results. More effective removal of the ambiguity requires more information about the sample, e.g. out of symmetry-plane information. Such data is evaluated by the approach of Benecke, et. al. [8] where generalized ellipsometric parameters are measured as a function of the angle of inclination for an azimuth of 45° with respect to the symmetry plane. From the subsequent numerical fitting to a suitable optics model [e.g. 16] the local refractive indices are obtained together with the director field across the LC-polymer film. A more simple and straightforward approach is based on evaluation of the transmittance of the retarder located between crossed polarizers as a function of light propagation (see fig. 9, left). Such a procedure has already been sketched by Vermiersch et. al. [9] but no automated parametrized fitting has been used in that paper and only approximate values were given as results for the birefringence of the layers.

The evaluation of the local refractive indices of compound retarders together with the director field from the measured transmittance of a sample retarder between crossed polarizers however includes some difficulties that have to be considered, e.g.: (1) normalization of the transmittance taking into account non-ideal effects of e.g. glass-substrates used (absorption), reflections at the interface glass-air and other interfaces,

(2) non-ideal polarizers (PVA-iodine layer between TAC-layers, see fig. 5b), and

(3) non-ideal alignment of the geometry (crossed polarizers and retarder to polarizers), etc..

Additionally, the transmittance is a highly non-linear function of the parameters of the model and of the direction of light propagation, and in order to obtain fast and secure convergence towards the global solution of the problem, suitable combinations

![Figure 10: Variation of the monochromatic transmittance of a compound retarder with a discotic layer (with linear tilt) and a TAC-layer (fig. 5a) with inclination of light propagation within the plane perpendicular to the plane of symmetry for various values of the refractive index, $n_a$, over a range of 0.05.](image1)

![Figure 11: Variation of the monochromatic transmittance of a compound retarder with a discotic layer (with linear tilt) and a TAC-layer (fig. 5a) with inclination of light propagation within the plane perpendicular to the plane of symmetry for various values of the refractive index, $n_a$, over a range of 0.05.](image2)

![Figure 12: Variation of the monochromatic transmittance of a compound retarder with a discotic layer (with linear tilt) and a TAC-layer (fig. 5a) with inclination of light propagation within the plane perpendicular to the plane of symmetry for various values of the refractive index, $n_a$, over a range of 0.05.](image3)
of parameter values have to be chosen as illustrated in figs. 10, 11 and 12. These figures illustrate the variation of transmittance with the local refractive indices for a range of inclination of light propagation between -60° and +60° in the plane that is located perpendicular to the plane of incidence (i.e. horizontal plane in the polar diagrams of fig. 9). For certain ranges of the angle of inclination there is at least a monotonous relation between the refractive index and the transmittance (see e.g. the ranges marked by the arrows), whereas for other angles of inclination there is no variation at all (see fig. 12, +20° < θ < +80°) or non-monotonous variations with reversal of direction (see fig. 11, 0° < θ < +80°).

In order to fill the currently existing gap between missing and non adequate data for key components of advanced LCDs and the increasing need for them, DIMOS, is being upgraded with a series of tools for systematic evaluation of optical data of key components of LCDs e.g. polarizers, retarders and other optical layers via numerical fitting of the measured directional distribution of transmittance to detailed optical models of the respective component [1].

4 Conclusions
We have shown that data often communicated for characterization of complex retarder sheets (i.e. layer retardations Δn_x, Δn_y) can vary to a considerable extent (up to almost 10%) due to assumptions made on the refractive index of the TAC-layer and that they are less depending on the model of the retarder used for the evaluation. Even a simple model used in the fitting process yields acceptable results.

Data currently available for characterization of complex retarders and polarizers is not sufficient for detailed numerical modeling and optimization of advanced LCDs where local complex indices of refraction versus wavelength of light and director distributions are needed instead of just birefringence values. In order to provide the user of numerical modeling software with the required data, tools have to be made available for evaluation of the target quantities from simple measurements, e.g. transmittance versus direction of light propagation.

The measurements and evaluations presented in this paper imply that the directional distribution of transmittance provides sufficient characteristic features in order to form the basis for a numerical evaluation of the local refractive indices and director distributions of the individual layers of compound retarders by automated parametrized fitting to a suitable optics model [1].

5 Acknowledgements
The discussions with Henning Wöhler and his expert advice are highly appreciated. Measurement and evaluation of the directional distribution of retarder transmission by Jürgen Laur is gratefully acknowledged. All numerical evaluations required for this paper have been carried out with DIMOS.

6 References
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