Retrieval of Liquid Crystal Director Profile from Optical Transmittance Measurements: A Case Study of Inverse-Problem in Optics with Layer Structures

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We develop an inverse-problem mathematical approach to retrieve liquid crystal (LC) director profiles from optical transmittance curves. We propose a new regularization matrix based on a *priori* knowledge of LC, which allows us to successfully retrieve the LC director profiles even with noise-contaminating optical transmittance data spanning only a limited range of incident angle. We demonstrate the functionality on two differently aligned LC cells biased at a variety of applied voltages. We show the technique to be useful for the design of optical devices with layer structures.

1. INTRODUCTION

The functionality of an optical device is usually yielded from the interaction of light with the device medium. One can further improve the device performance by tailoring the distribution of material property along the optical propagation direction for accumulating the effect of the light-matter interaction. On the other hand, for the concern of material characterization, the optical field after passing through a material may carry useful information about the material structure [1]. Optical tomography [2–4] represents an inspiring example of the concept. Direct determination of a material structure from measured optical responses lies in the category of inverse problem [5–8], which is difficult to be resolved and has produced very few cases of success.

To facilitate further discussion, we will focus on optical devices with layered structures, which had been widely used in many applications. Retrieving the depth profile of refractive index of a device from optical transmittance data is ill-posed [9–12], which prevents us from deducing the profile accurately and reliably [1, 13]. To cope with the difficulty, researchers in the past favored the forward-problem simulation approach to deduce the model parameters. However, there are many systems whose mathematical models are either unavailable or inaccurate enough for the purpose. It is therefore of great interest to improve the technique of the inverse problem approach and verifies its applicatbility on optical devices.

In this paper, we developed an inverse-problem approach to retrieve the refractive index profile of an optical device with layered structure. Our method employs a general formalism of light propagation in an optical medium and no model of layer structure is needed. Therefore, our retrieval methodology is essentially model free. To test its applicatbility, we particularly chose liquid crystal (LC) in viewing that the continuum medium model of LC had been shown to be accurate. It is therefore approriate to apply the continuum medium model of LC to verify the results with our inverse-problem retrieval technique. We proposed a regularization matrix based on a *priori* knowledge of LC to improve the retrieval reliability. We demonstrated the functionality of our method on two differently aligned LC cells biased at a variety of applied voltages. We successfully applied the technique to retrieve LC director profiles even with noise-contaminating optical transmittance data which span only a limited range of incident angle. The results presented in this paper indicate our method to be widely applicable for optical devices with layer structures.

2. THEORETICAL DETAILS

Inverse problem is ill-conditioned, and therefore not amenable to direct matrix inverse techniques that typically reveal a disadvantage of noise amplification [14–17]. Several regularization methods had been proposed to solve this problem by using *prior* information to calculate an estimate. For an illustration, considering an image processing case $g = Hf + n$, where g and f are vectors of length m represents the measured and original images, respectively, H denotes an $m \times m$ linear operator that characterizes the image degradation, and n is a vector of length m that represents additive white noise contaminating the measurements. The goal is to solve for an acceptable estimate of the original image without excessive noise. To achieve the goal, Tikhonov regularization [14, 15] can be invoked to

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yield an image estimate $\hat{f}_{tik}$ that minimizes

$$\hat{f}_{tik}(\alpha) = \arg\min_{f} \|g - Hf\|^2 + \alpha \|L f\|^2 , \tag{1}$$

where $\|...\|$ implies L-2 norm. The first term measures the fidelity of the solution to the data while the second term measures the fidelity to the *prior* knowledge expressed in operator L. Here α controls the tradeoff between fidelity to measurements and to *prior* information [16, 17].

For the problem of LC, we must first devise a workable optical model to evaluate the optical transmittance of a LC film with a gien director profile $\theta(z)$. This can be done by converting $\theta(z)$ into a dielectric-constant profile $\varepsilon[\theta(z)]$ and then calculating the optical transmittance via the Berreman matrix method [18, 19]. The output optical field Ψ_{out}, depending on the dielectric profile, can be expressed as

$$\Psi_{out} = B[\epsilon(\theta)]\Psi_{in}, \tag{2}$$

where $B[\epsilon(\theta)]$ denotes the Berreman matrix. The dielectric tensor of a transperent uniaxial film can be properly described with a symmetric 3×3 matrix with six elements; whereas the corresponding optical axis of the film is fully determined by two components only. Therefore, to retrieve the dielectric profile of a layered structure from optical measurements, we have to solve an inverse problem with 6 unknown variables per layer [9]. This causes a significant complication. We abated the difficulty by developing an inverse problem formalism to retrieve the LC director profile directly from measured optical transmittance data.

We start with equation (2) and rewrite it as

$$\Psi_{out} = B(\theta_0)\Psi_{in} + \delta\Psi, \tag{3}$$

where $\delta\Psi$ denotes the difference of the optical field deduced from the optical measurements and the field from a properly estimated profile $\theta_0(z)$ with a given surface condition. To reveal further the mathematical details of the inverse problem in LC, we focused on $\delta\Psi$ and derived an equation to show how a director profile change affects $\delta\Psi$. We first invoked the Berreman matrix formalism [14, 15] to describe the wave propagation effect in LC with an ordinary differential equation

$$(\frac{d}{dz} + i\omega\Pi_\xi)\Psi_\xi = 0. \tag{4}$$

Here ξ denotes the incident angle of input light and $\Pi_\xi\,(\theta)$ is the differential propagation matrix. Note that a variation in pretilt angle can cause a change of Berreman matrix, which further varies the optical field vector Ψ. By taking this functional dependence into account and invoking the equation of equation (4), we then obtain

$$(\frac{d}{dz} + i\omega\Pi_\xi)\delta\Psi = -i\omega(\delta\Pi\Psi + \delta\Pi\delta\Psi). \tag{5}$$

Equation (5) is a differential equation. We can cast it into an operator form

$$L \cdot u = f, \tag{6}$$

where $L = (d/dz + i\omega\,\Pi_\xi)$, $u = \delta\Psi$, and $f = -i\omega(\delta\Pi\Psi + \delta\Pi\delta\Psi)$. Equation (6) has a solution

$$u = Hu(0) + G[f] \tag{7}$$

with G denoting the corresponding Green's function operator. By using the initial condition of $\mathbf{u}\,(0) = 0$, equation (5) can be rewritten as

$$\delta\Psi = -i\omega(1 + i\omega G\delta\Pi)^{-1}G[\delta\Pi\Psi] \cong -i\omega G[\delta\Pi\Psi], \tag{8}$$

where the Neumann series $(1 + i\omega G\delta\Pi)^{-1} = 1 + (-i\omega G\delta\Pi) + (-i\omega G\delta\Pi)^2 + ...$ is kept up to the first-order term in viewing that $\|\omega\, G\,\delta\Pi\| \ll 1$. We can convert the Green's function to an integral form and transform equation (8) into an integral equation

$$\delta\Psi(d) = -i\omega\int_0^d g(d,z)\delta\Pi(z)\Psi(z)\,dz. \tag{9}$$

By substituting $\Psi(z) = e^{-i\omega\Pi z}\Psi(0)$ and $g(d,z) = e^{-i\omega(d-z)\Pi}$ into equation (9), we obtain

$$\begin{aligned}\delta\Psi\left(d\right) &= -i\omega\int_0^d e^{-i\omega(d-z)\mathbf{\Pi}}\delta\Pi\left(z\right)e^{-i\omega z\mathbf{\Pi}}\ \Psi(0)dz \\ &= -i\omega\ e^{-i\omega d\,\Pi}\int_0^d e^{i\omega z\mathbf{\Pi}}\delta\Pi\left(z\right)e^{-i\omega z\,\mathbf{\Pi}}\ \Psi(0)dz.\end{aligned} \tag{10}$$

Since equation (10) is an integral form, a data set covering a wider range of incident angle would carry more information and therefore yields a tighter constraint on the solution. Furthermore, equation (10) is essentially a Fourier transform and can easily generate an oscillation in the director profile during the LC inverse problem retrieval procedure.

Ψ is a functional of pretilt angle profile $\theta(z)$. By decomposing the LC film into a sequence of layers with $\theta(z)_{z=z_1,z_2,...,z_n} = \theta_1,\theta_2,...,\theta_n$, the output field from the LC film can be approximated to be

$$\Psi_{out}(\theta_1,\theta_2,...,\theta_n) = B(\theta_1,\theta_2,...,\theta_n)\Psi_{in}. \tag{11}$$

The optical field variation by a change in the pretilt angle profile is given by

$$\begin{aligned} d\Psi &= J\,d\theta \\ &= \left(\frac{\partial B}{\partial\theta_1}d\theta_1 + \frac{\partial B}{\partial\theta_2}d\theta_2 + ... + \frac{\partial B}{\partial\theta_n}d\theta_n\right)\Psi_{in},\end{aligned} \tag{12}$$

where J denotes the Jacobian matrix $J_{ij} = \dfrac{\partial B_i}{\partial\theta_j}$. Although Ψ carries the complete information about the amplitude and phase of an optical wave, the noise influence on the phase of Ψ will be amplified and seriously degrades the accuracy of a solution. To avoid the difficulty, we transformed the equation in the field representation to the intensity representation. This can be done by separating $\partial\Psi/\partial\theta$ into the real and the imaginary part

$$\frac{\partial\Psi}{\partial\theta} = \frac{\partial(Re\Psi)}{\partial\theta} + i\frac{\partial(Im\Psi)}{\partial\theta}. \tag{13}$$

The derivative of optical intensity with pretilt angle can be written as

$$\frac{\partial I}{\partial\theta} = 2(Re\Psi)\cdot\frac{\partial(Re\Psi)}{\partial\theta} + 2(Im\Psi)\cdot\frac{\partial(Im\Psi)}{\partial\theta}. \tag{14}$$

Fig. 1 depicts the flowchart of our approach. The iteration process begins with an initial director profle estimated from either a linear interpolation or a more accurate simulated result with given surface alignment consitions. Equation (12) and equation (14), and the associated Jacobian matrices form the mathematical ground to solve the inverse problem of LC director profile [20].

3. EXPERIMENTAL APPARATUS FOR THE LC INVERSE PROBLEM RETRIEVAL

As shown in Fig. 2, an apparatus was set up to acquire the optical transmittance data for the inverse problem retrieval of LC profile. We used a He-Ne laser with a wavelength of 633 nm as the light source. The optical transmittance measurements were resolved into x- and y-component with an analyzer T and detected with a CCD camera. The incident light was arranged in four different polarization states by using a combination of a polarizer and a quarter-wave plate. The four polarization states are comprised of three linearly polarized light at 22.5°, 67.5° and 112.5° to the laboratory x-axis, respectively, and one left circularly polarized light. A rotation stage was used to vary the incident angle into the LC cell to cover a range from −50° to 50°.

A 4 μm-thick planar alignment LC cell with 1° pretilt is used for the test run. The director profile of the LC cell is generated with Q-tensor approach [21] implemented with a finite element partial differential equation (PDE) solver. The optical transmittance of the LC cell was calculated with an optical model based on the Berreman matrix method. The test run aims to investigate the influences of data regularization, noise, and finite range of incident angle on the LC inverse problem retrieval.

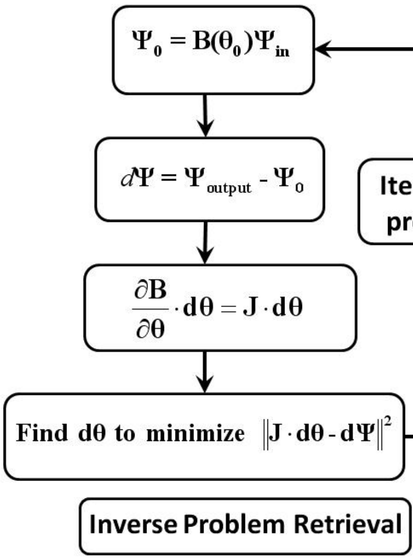


FIG. 1: The flowchart used to search for the LC director profile with given optical transmittance measurements.

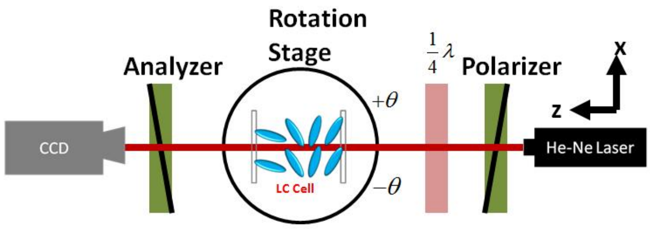


FIG. 2: Experimental setup used to measure the optical transmittance data for inverse problem retrieval of LC director profile.

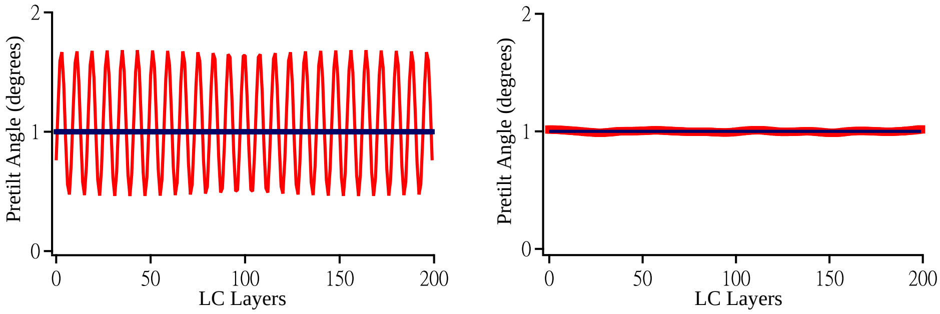
4. SIMULATION RESULTS

To illustrate the importance of data regularization for an inverse problem, we first set up a simulation by adding a noise level of 1% to the simulated transmittance data and retrieved the LC director profile with the Tikhonov regularization scheme [16]. The regularization parameter was single constant and optimized with the L-curve approach [16]. Figure 3(a) presents the retrieved LC director profile with red solid curve, showing a fairly strong oscillation from noise influence since noise in the data can be amplified and seriously degrades the reliability of the retrieved solution. By comparing to the true LC director profile (blue solid curve) from our PDE solver, the Tikhonov regularization with single regularization parameter apparently does not yield a satisfactory result.

To minimize the oscillatory behavior, we designed a new data regularization scheme. This new method exploits some *prior* knowledge on the physics of LC, which demands LC profile to be continuous without an abrupt variation. We implemented the *prior* knowledge into the data regularization of equation (1) with a new form of matrix L. A proposed regularization matrix appropriate to our application is shown below

$$\alpha L = \begin{bmatrix} \alpha & 0.1\alpha & 0.01\alpha & 0 & 0 & ... & ... \\ 0.1\alpha & \alpha & 0.1\alpha & 0.01\alpha & 0 & 0 & ... \\ 0.01\alpha & 0.1\alpha & \alpha & 0.1\alpha & 0.01\alpha & 0 & ... \\ 0 & 0.01\alpha & 0.1\alpha & \alpha & 0.1\alpha & 0.01\alpha & ... \\ 0 & 0 & 0.01\alpha & 0.1\alpha & \alpha & 0.1\alpha & ... \\ 0 & 0 & ... & ... & ... & ... & ... \\ ... & ... & ... & ... & ... & ... & ... \end{bmatrix}. \quad (15)$$

The choice is reasonable in viewing that each LC molecule shall experience a constraint that depending on the distance to its neighoring molecules. To further avoid oscillation in the iteration, a small step size was used at the begining stage and when the solution was sufficiently close to the correct answer, the retrieval procedure then took

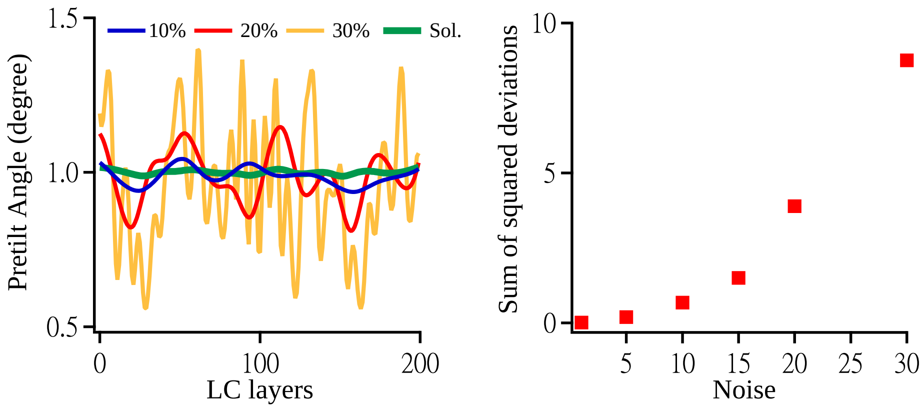


(a) (b)

FIG. 3: Comparison of the retrieved LC director profiles by using different regularization methods. The transmittance data were prepared with the finite element simulation based on Q-tensor approach and then added with one percentage of noise. (a) LC director profile retrieval by using single-parameter Tikhonov regularization scheme. (b) LC director profile retrieval by using our new regularization method.

larger step sizes. Figure 3(b) displays the retrieved LC director profile with this new method, revealing a highly efficient suppression of the intrinsic oscillating behavior in the inverse problem retrieval.

To test the robustness of our inverse problem procedure, we added 1% to 30% noise level to the data from simulation on a 4 μm-thick planar alignment LC cell with 1^o pretilt angle. The results are presented in Figure 4(a). It is exciting to find that even at 10% noise level the retrieved profile (blue curve) agrees well with the true profile shown with the green line. The averaged pretilt calculated from the retrieved profiles with 1%, 5%, and 10% noise level are 1^o, 0.99^o, and 1.01^o, respectively. The summation of squared deviations of the retrieved profiles from the true profile as a function of the noise level is shown in Figure 4(b), revealing that the root-mean squared deviation per data point can be as small as 0.02^o even with 30% noise level.



(a) (b)

FIG. 4: LC director profiles retrieved from the transmittance data. The data are prepared first with the finite element simulation based on Q-tensor approach and then added with 1%, 5%, 10%, 15%, 20%, 30% of noise. (a) The retrieved LC director profiles. (b) The summation of absolute squared deviations of the retrieved profiles from the true profile as a function of the noise level added.

To successfully retrieve a LC director profile, the data set of optical transmittance shall cover a range of incident angle as wide as possible. However, regarding about how wide the range is sufficient to yield a reliable result does not have a clear answer. We follow the previous example and proceed to analyze the effect of finite range of incident angle. Three data ranges with I ($-10^o \rightarrow 10^o$), II($-30^o \rightarrow 30^o$), and III($-50^o \rightarrow 50^o$) were chosen. Each set of simulated optical transmittances were contaminated with 5% noise level. Fig. 5 presents the retrieved LC director profiles from the three sets of data. We found that the LC director profiles from the data sets I (light green color) and II (blue color) periodically deviate from the true profile (light brown color) by about 1.85^o and 0.72^o, respectively, originating clearly from insufficient information for the inverse problem retrieval. The data set III does yield a satisfactory profile even with noisy input data which containing 5% noise.

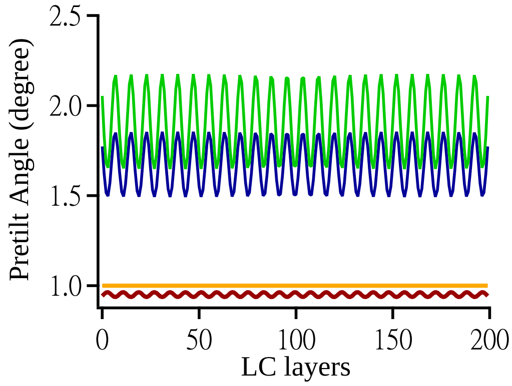


FIG. 5: The retrieved LC director profiles from three sets of simulated optical transmittance data: I (-10^o $\rightarrow$ 10^o: light green color), II(-30^o $\rightarrow$ 30^o: blue color), and III(-50^o $\rightarrow$ 50^o: brown color). The true profile (light brown color) is also included for comparison.

5. INVERSE PROBLEM RETRIEVAL OF LIQUID CRYSTAL DIRECTOR PROFILE FROM OPTICAL TRANSMITTANCE MEASUREMENTS

As indicated in equation (2), the model parameters can be connected with the measured data through a linear mapping. Therefore, a linear inverse problem solver [20] could be a proper choice for the determination of a model from measured data. To demonstrate the functionality of the inverse problem solver, we retrieved the director profiles of two LC cells from the optical transmittance measurements. The LC cells used are a 4 μm-thick LC cell with hybrid alignment and a 4 μm-thick optically compensated bending (OCB) LC cell in a splay mode.

The polarization-resolved optical transmittance measurements of the hybridly aligned LC cell are presented in Figure 6 and Figure 7 with an applied voltage of 0V and 5V, respectively. The x- and y-direction-resolved optical transmittances with an input light polarized at four different polarization states were measured. The measured optical transmittances (filled symbols) are then compared with the simulation curves (solid lines). Deviations between the two curves were used to adjust the LC director profile during the inverse problem retrieval process.

Figure 8 shows the retrieved LC director profiles for the hybrid cell with three applied voltages of 0V, 2.5V, and 5V. For a clear comparison, two LC director profiles are plotted together: one profile (blue solid curves) was obtained from the FEM simulation on the LC cell [22], and the other profile with red filled symbols was retrieved from the optical transmittance measurements with our inverse problem retrieval technique. Note that the inverse problem retrieval technique always converge to an almost identical result no matter what an initial director profle from a linear interpolation or a simulated result with given surface pretilt angles is used. Although weak oscillations remain in the retrieved profile at nonzero applied voltages, the overall agreement between the retrieved and the simulated profiles is fairly good.

Similar measurements had also been performed on an OCB cell. Figure 9 exhibits the results of the OCB cell. Similarly, our inverse problem retrieval converges to an identical result no matter what an initial director profle from a linear interpolation or a simulated result is used. The overall agreement between the retrieved and the simulated profiles is excellent, indicating that our inverse problem retrieval technique is robust and accurate enough for a practical application.

For a layered structure of liquid crystal, the model parameters can be retrieved with non-linear inverse problem technique. The resulting converging rate was found to be $O(\sqrt{\delta})$ [23], where δ is the norm bound $\|g - Hf\| \leqslant \delta$ defined in equation (1). However, by using a linear inverse problem solver, a proper choice of regularization matrix (αL) can lead to a faster converging rate $O(\delta^{2/3})$ [24].

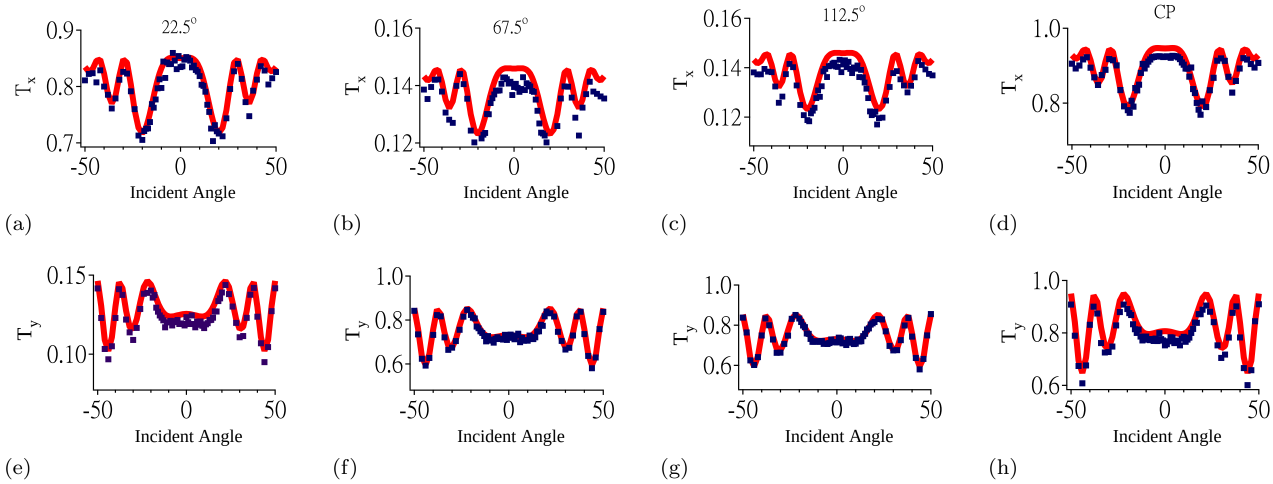


FIG. 6: The polarization-resolved optical transmittance measurements T_x and T_y of a LC cell with hybrid alignment are presented by using four different input polarization states (22.5^o, 67.5^o, 112.5^o, and CP). The LC cell was driven with an applied voltage of 0V. Two curves are included for comparison, red solid curves: simulated results with Berreman matrix technique, and filled symbols: the optical transmittance measurements as a function of incident angle.

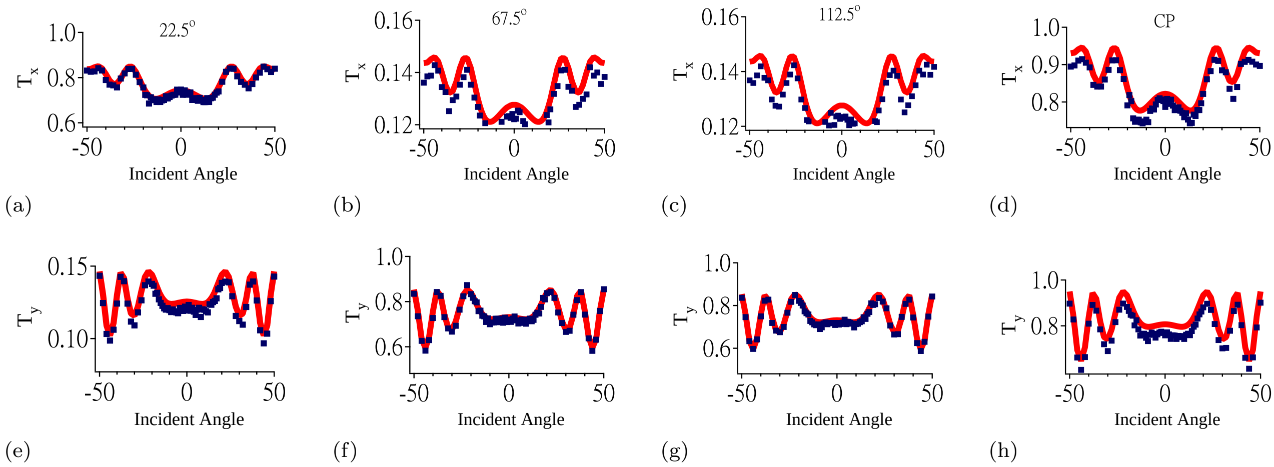
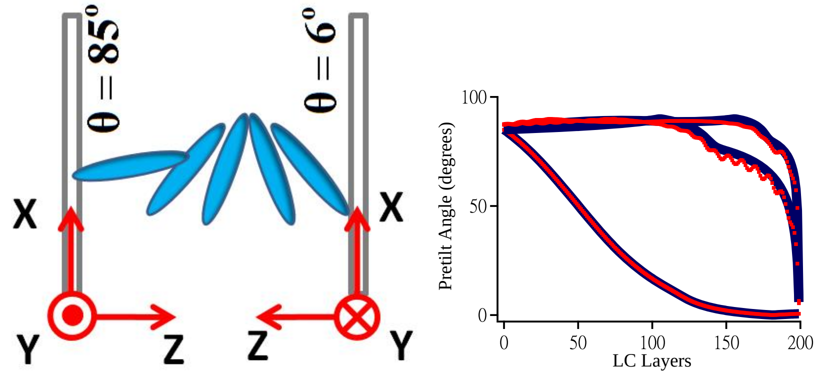


FIG. 7: The polarization-resolved optical transmittance measurements T_x and T_y of a LC cell with hybrid alignment are presented by using four different input polarization states (22.5^o, 67.5^o, 112.5^o, and CP). The LC cell was driven with an applied voltage of 5V. Two curves are included for comparison, red solid curves: simulated results with Berreman matrix technique, and filled symbols: the optical transmittance measurements as a function of incident angle.

As shown by equation (12) a variation in the pretilt angle profile can cause a change in the optical field. Based on the multi-layer model of liquid crystal cell, the regularization matrix of equation (15) indicates the field in j layer can be affected by its nearest neighboring layers with Jacobian coupling element inversely depending on the distances. We assume ten times weaker per layer in the elements of equation (15). However, it shall be noted that further improvement of the performance shall be possible by tailoring the regularization matrix with *prior* knowledge from more detailed simulation results.

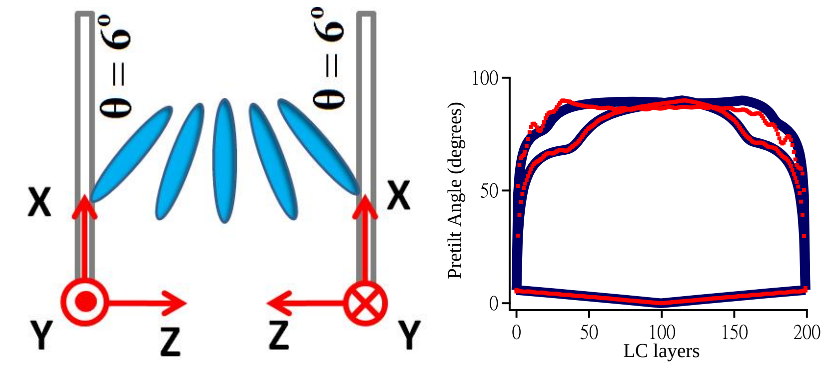
6. CONCLUSION

We developed an inverse problem method to retrieve LC director profile from optical transmittance measurements by deriving the equations and detailed steps involved. We proposed a regularization matrix based on a *priori* knowledge of LC to minimize an intrinsic oscillating behavior in the director profile during the LC inverse problem retrieval procedure. This new regularization matrix allows us to robustly retrieve LC director profiles with noisy



(a) (b)

FIG. 8: The retrieval director profiles of a hybrid cell by our inverse problem retrieval method. (a) The coordinate system used to present the LC director profiles. (b) The retrieved director profiles of the hybrid cell biased at 0V, 2.5V, and 5V. Two profiles are included for comparison: the curves of red filled squares: retrieved profile directly from optical transmittance measurements, and blue solid curves: the simulated profile calculated by the FEM with Q-tensor approach.



(a) (b)

FIG. 9: The retrieval director profiles of an OCB cell by our inverse problem retrieval method. (a) The coordinate system used to present the LC director profiles. (b) The retrieved director profiles of the OCB cell biased at 0V, 2.5V, and 5V. Two profiles are included for comparison: the curves of red filled squares: retrieved profile directly from optical transmittance measurements, and blue solid curves: the simulated profile calculated by the FEM with Q-tensor approach.

optical transmittances of LC cells measured in a finite range of incident angle and with various applied voltages. The results indicate our method to be useful for the design of LC devices where the director profiles needed to be carefully tailored.

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7. REFERENCES

[1] J.-M. Tualle, H. L. Nghiem, D. Ettori, R. Sablong, E. Tinet, and S. Avrillier, J. Opt. Soc. Am. A **21**, 24 (2004).
[2] G. Bal and J. C. Schotland, PRL **104**, 043902 (2010).
[3] A. D. Klose and A. H. Hielscher, opt. Lett. **28**, 1019 (2003).
[4] G. Bal, A. Jollivet, and V. Jugnon, nverse Problems **26**, 025011 (2010).
[5] P. G. de Gennes and J. Prost, *The physics of liquid crystals* (Oxford University Press, 1993).
[6] G. Bal, Inverse Problems **25**, 053001 (2009).

[7] A. Tarantola, *Inverse problem theory and methods for model parameter estimation* (SIAM: Society for Industrial and Applied Mathematics, 2005).
[8] A. G. Ramm, *Inverse Problems: Mathematical and Analytical Techniques with Applications to Engineering* (Springer, 2005).
[9] W. R. B. Lionheart and C. J. P. Newton, New J. Phys. **9**, 63 (2007).
[10] S. L. Cornford, T. S. Taphouse, C. J. P. Newton, and J. R. Sambles, New J. Phys. **9**, 166 (2007).
[11] A. N. Tikhonov, Dokl. Akad. Nauk SSSR **39**, 195 (1943).
[12] A. N. Tikhonov, *Solution of ill-posed problems* (Vh Winston, 1977).
[13] G. Alexandrakis, D. R. Busch, G. W. Faris, and M. S. Patterson, Appl. Opt. **40**, 3810 (2001).
[14] P. C. Hansen, BIT Numer. Math. **30**, 658 (1990).
[15] A. Neumaier, SIAM Review **40**, 636 (1998).
[16] A. M. Thompson, J. C. Brown, J. W. Kay, and D. M. Titterington, IEEE tran. PAMI **13**, 326 (1991).
[17] C. Gu, Inverse Problems **24**, 034002 (2008).
[18] D. W. Berreman, J. Opt. Soc. Am. **62**, 502 (1972).
[19] T. Scharf, *Polarized light in liquid crystals and polymers* (Wiley-Interscience, 2007).
[20] *Fortran Linear Inverse Problem Solver (FLIPS)*.
[21] N. J. Mottram and C. J. Newton, *Introduction to Q-tensor theory*, Tech. Rep. (Tech. Rep. 10/04 University of Strathclyde, 2004).
[22] P. G. Ciarlet, *The finite element method for elliptic problems* (SIAM: Society for Industrial and Applied Mathematics, 2002).
[23] H. W. Engl, K. Kunisch, and A. Neubaue, Inverse Problems **5**, 523 (1989).
[24] A. Neubauer, Appl. Num. Math. **4**, 507 (1988).