Optics Communications ∎ (∎∎∎∎) ∎∎∎–∎∎∎

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Accurate transmittance analysis of liquid crystal displays using a rational fraction approach in the time domain

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ARTICLE INFO

Article history:
Received 11 February 2015
Received in revised form
13 April 2015
Accepted 24 April 2015

Keywords:
Liquid crystal display
Finite-difference time-tomain method
Rational fraction approach
Multi-pole fitting

ABSTRACT

Transmittance of liquid crystal display (LCD) is accurately characterized by using a rational fraction approach to extract complex multi-poles corresponding to a modified Drude–Lorentz dispersive model in the time-domain simulation. Here, the multi-pole fitting accuracy to the measured complex refractive indices of color filters and polarizers with low absorption coefficients and high noise levels is significantly improved with suggested multi-pole fitting algorithm. Then, the transmittance and power distribution of LCD for oblique incidence are analyzed with high angle accuracy, and the color shift arising from the misalignment between the color filter and thin-film transistor substrates is effectively evaluated.

1. Introduction

The finite-difference time-domain (FDTD) computation [1–3] of Maxwell's equations has been widely used as an efficient simulation tool to successfully predict lightwave propagation within liquid crystal (LC) devices [4–9]. Here, the FDTD method can simulate the complex anisotropic LCs by considering strong scattering and diffractive effects due to the rapid LC variation as well as spatial inhomogeneties of the LC director orientation, while the commonly used matrix methods are limited by specific types of geometries in modeling anisotropic structures [10,11]. To implement frequency responses of dispersive materials in the time-domain method, one needs to accurately and efficiently incorporate real material dispersions by fitting a given permittivity function as the sum of multiple Debye or Lorentz pole pairs. Thus, various material dispersion models such as Debye [12], Drude–Lorentz [13,14], and extension of Lorentz [15], have been used to date. Although these multi-pole models show good fit to the measured data, the number of poles required for the fitting become quite large, resulting in significant increase in memory and computational costs. Thus, by replacing a set of starting poles with an improved set of poles via a scaling procedure, a rational function approximation [16,17] has been adopted to fit measured frequency-domain responses. This method extends the functions with a high number of resonance peaks by allowing complex starting poles [18]. Also, attempts toward more unified description using Drude term followed by critical points have been reported [19–21].

Meanwhile, since k-values (imaginary part of complex index) in a transmission range of color filter (CF) and those in a transmission axis of polarizers are very low with high noise levels during measurements, there always exists an issue of properly measuring the refractive indices of CF and polarizer in a liquid crystal display (LCD). Especially, a large variation of refractive index with much noise occurs for low k-values, and high transmission property of these materials also tends to reduce the fitting capability in a visible wavelength range. Thus, it is difficult to extract the solutions of electromagnetic simulation completely satisfied with all the measured data of these dispersive materials through the normal fitting procedure because lots of poles should be generated for the CF and the polarizer. Furthermore, they are so sensitive to the variation of the measured data that there exists an increased chance of simulation failure. Therefore, we need to find *a* new approach capable of increasing the fitting stability and accuracy through simplifying the data for these dispersive materials.

Thus, in this paper we firstly adopt a rational fraction approach [18] combined with a new multi-pole fitting algorithm to extract complex multi-poles corresponding to the coefficients of modified Drude–Lorentz model for the FDTD simulation of LCDs. Then, the transmittance characteristics are systematically investigated by varying incident angle of lightwave propagating through the dispersive materials such as polarizers, LCs, and CF layers with high angle accuracy. In addition, the degree of color shift for the LCD

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http://dx.doi.org/10.1016/j.optcom.2015.04.064
0030-4018/© 2015 Published by Elsevier B.V.

panel depending on the amount of misalignment between the CF and TFT-substrates is efficiently estimated on the CIE (the Commission Internationale de l'Eclairage)-xyY color space, which consequently allows us to characterize the display performance.

2. A rational-fraction dispersion approach

A rational-fraction dispersion approach uses complex form of multi-poles to estimate the coefficients of the modified Drude–Lorentz model described by

$$\varepsilon = \varepsilon_\infty + \sum_{p=1}^{P} \frac{\omega_p^2 - i\gamma_p'\omega}{\omega_{0p}^2 - i\gamma_p\omega - \omega^2} \tag{1}$$

where ε_∞, ω_p, ω_{op}, γ_p, and $\gamma_p{}'$ are the relative permittivity at infinite frequency, the plasma frequency, the resonance frequency, the damping factor, and the fitting parameter, respectively. By considering two complex fraction terms of complex conjugate residues and pole pairs, Eq. (1) can be generalized by the Drude terms followed by critical point scheme [20] as

$$\varepsilon = \varepsilon_\infty + \sum_{p=1}^{2P} \frac{c_p}{d_p - \omega} \tag{2}$$

where the residue (c_p) and the pole (d_p) are fitting coefficients that do not necessarily have any physical meaning. Then, the dispersive material's relative permittivity can be represented by the rational fraction form [18] as

$$\varepsilon = \frac{\sum_{p=0}^{2P} a_p\,\omega^p}{\sum_{p=0}^{2P} b_p\,\omega^p} \tag{3}$$

or a global matrix form as

$$\begin{pmatrix} \omega_0^0 & \omega_0^1 & \cdots & \omega_0^{2P} & -\varepsilon_0\omega_0^0 & -\varepsilon_0\omega_0^1 & \cdots & -\varepsilon_0\omega_0^{2P} \\ \omega_1^0 & \omega_1^1 & \cdots & \omega_1^{2P} & -\varepsilon_1\omega_1^0 & -\varepsilon_1\omega_1^1 & \cdots & -\varepsilon_1\omega_1^{2P} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \omega_N^0 & \omega_N^1 & \cdots & \omega_N^{2P} & -\varepsilon_N\omega_N^0 & -\varepsilon_N\omega_N^1 & \cdots & -\varepsilon_N\omega_N^{2P} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{2P} \\ b_0 \\ b1 \\ \vdots \\ b_{2P} \end{pmatrix} = 0 \tag{4}$$

It is noted that the number of measured data is always larger than that of poles in the equation. The parameters a_p and b_p of the two polynomials in Eq. (3) were obtained by a rational approximation method and employed as *a* good initial guess for the curve fitting of material permittivity. Here, we fixed some parameters of a_p and b_p according to the measured data and use the symmetry of the permittivity function. The initial values of the residues, poles, and direct coefficient ε_∞ obtained from the a_p and b_p were used in a simulated annealing algorithm [22] to find the optimized values of parameters. Thereafter, the coefficients of modified Drude–Lorentz models were estimated along the principle axes of a second rank dielectric tensor of LC material to perform the FDTD simulation of LCDs.

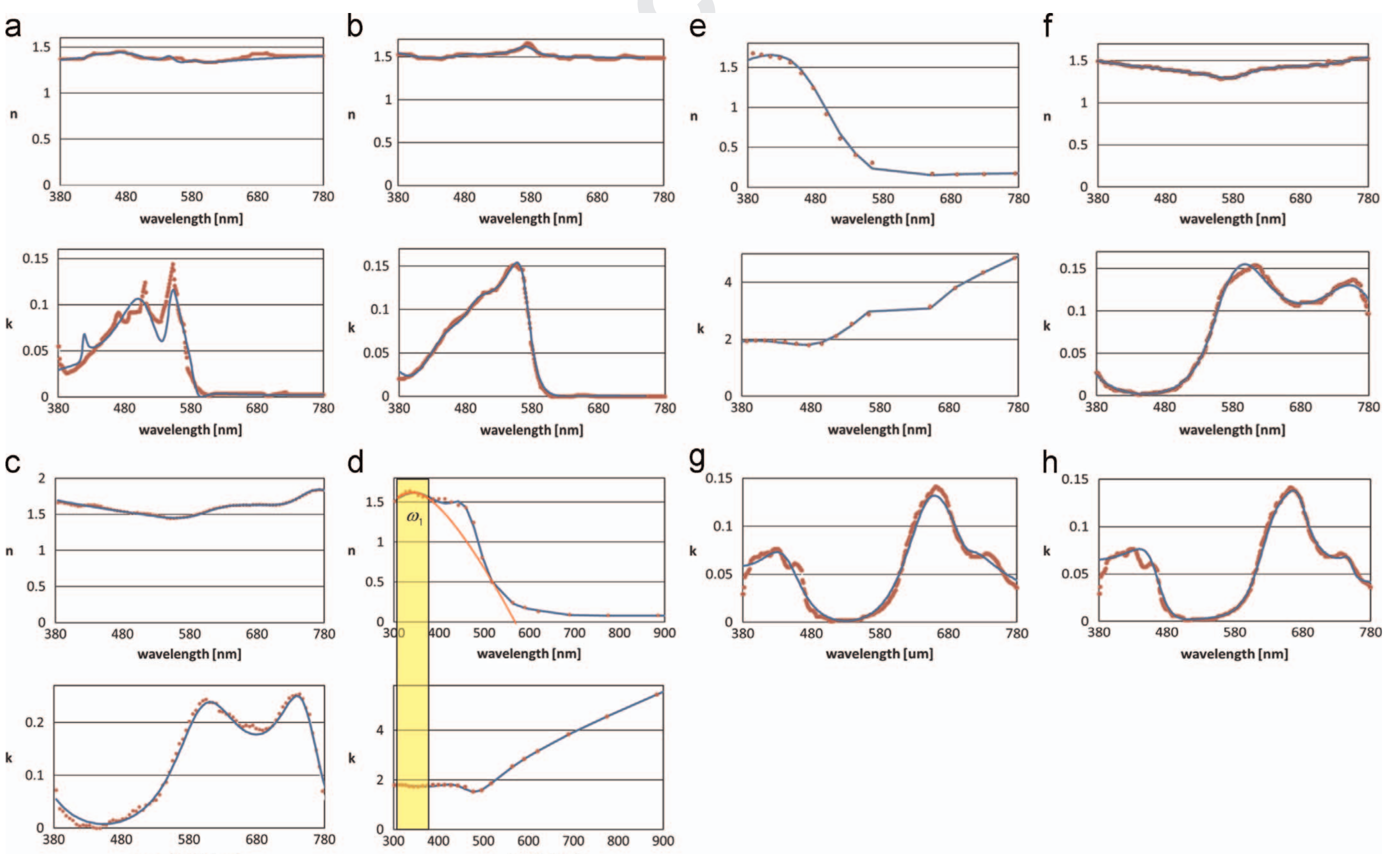

Fig. 1. The fitted real (n) and imaginary (k) values of refractive indices (blue lines) with respect to the measured n- and k- values (red dots), showing improved fitting accuracy by suggested fitting algorithm using (a) average smoothing, (b) noise reduction, (c) weight smoothing, (d) extending wavelength region for fitting, (e) threshold smoothing, (f) extracting procedure of proper n-, k- values, (g) and (h) fitting for higher order poles. Here, the materials used for fitting were R-CF in (a) and (b), B-CF in (c) and (f), G-CF in (g) and (h), and gold metal in (d) and (e). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)