Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

FDTD Method for Light Interaction with Liquid Crystals

V. Ilyina* [a], S. J. Cox [a] & T. J. Sluckin [b]

[a] School of Engineering Sciences, University of Southampton

[b] School of Mathematical Sciences, University of Southampton

Version of record first published: 18 Oct 2010

To cite this article: V. Ilyina*, S. J. Cox & T. J. Sluckin (2004): FDTD Method for Light Interaction with Liquid Crystals, Molecular Crystals and Liquid Crystals, 422:1, 1-10

To link to this article: http://dx.doi.org/10.1080/15421400490501932

Mol. Cryst. Liq. Cryst., Vol. 422, pp. 1/[271]–10/[280], 2004

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421400490501932

Taylor & Francis
Taylor & Francis Group

FDTD METHOD FOR LIGHT INTERACTION WITH LIQUID CRYSTALS

V. Ilyina and S. J. Cox*
School of Engineering Sciences, University of Southampton

T. J. Sluckin
School of Mathematical Sciences, University of Southampton

Finite-difference time domain method (FDTD) for optical propagation through liquid crystal structures have been compared with analytical results. Conclusions about the accuracy of the FDTD method and possible sources of errors have been made. An algorithm that provides feedback between the change of the director distribution and the optical field has been proposed. We have demonstrated the effectiveness of our technique by considering the example of light propagation through a nematic liquid crystal cell with an applied electric field and photosensitive polymer on one of the substrates. The results give insight into the demands of the FDTD method for liquid crystal structures and demonstrate how it might be extended for more complex liquid crystal devices.

Keywords: FDTD method; optics of liquid crystals

INTRODUCTION

Modelling of light interaction with liquid crystals has been always important for designing light-responsive liquid crystal devices. During the early years of developing liquid crystal technology, several methods were designed to study light propagation through liquid crystal structures. These methods, such as Berreman matrices and the extended Jones method [1,2] have been successfully employed for optical analysis of one-dimensional director structures. However, recent advances in liquid crystal device technology make it necessary to develop more advanced numerical methods to allow realistic devices to be modelled. These methods should be able to accommodate liquid crystal structures that can contain multiple domains, possess significant multidimensional spatial inhomogeneities of the director, or interact with several beams.

*Correspondence author. Tel.: +44 (0)23 80593390, E-mail: v.ilyina@soton.ac.uk

All these cases require accurate calculation of reflected and scattered fields and propagation of oblique incident light through liquid crystal structures with director variations in more than one dimension.

The finite-difference time-domain (FDTD) [3] computation of Maxwell's equations for light propagation in liquid crystal medium has been considered for the optical analysis of structures that can not be examined by matrix methods. FDTD method gives full information about transmitted, reflected and scattered fields and does not require simplifying assumptions about the director distribution. Another advantage of the method is the explicit time scheme that allows one to follow the interaction of light with the system over time and make observations about its time response.

However, despite the advantages of the FDTD method, one should not forget that it provides only a numerical approximation of the solution to Maxwell's equations. It is important to carefully check the accuracy of the solution against analytical or other computational solutions [4]. Our long term goal is to model accurately light interaction with liquid crystal devices possessing complex variations in the director. In this paper we compare FDTD results with known methods and introduce the algorithm for time-dependent problem.

We first introduce the basics of the FDTD method for dielectric anisotropic medium. We go on to make comparison of FDTD method data with the matrix method results. Finally we introduce the algorithm for following the interaction of light with the liquid crystal cell with polymer layer over time and make observations about its time response.

LIQUID CRYSTALS AND FDTD METHOD

The FDTD method allows us to solve numerically Maxwell's equations for light propagating through liquid crystal structures. Time evolution in FDTD calculation is represented by a leapfrog scheme and a staggered grid for electric and magnetic fields composed of Yee cells is introduced for spatial discretisation [5]. Both space and time derivatives are approximated with central second order finite differences. To truncate the computational window Berenger's perfectly matched layer (PML) boundary conditions were chosen [4,6].

The important parameters for FDTD simulations are time step Δt and spatial discretisation Δh. Their choice influences the stability and accuracy of the method. The conventional upper bound for time step is:

$$\Delta t \leq \frac{\Delta h}{v}, \tag{1}$$

where $v = c/n$ is the phase velocity of wave in the medium, c being the light velocity and n the refractive index. The relationship (1) means that

during one time step the wave can propagate not more than one spatial cell. If it turns to equality, the wave propagates exactly one cell and the solution is exact and does not suffer numerical dispersion [3]. However, since a liquid crystal has a spatially varying anisotropic dielectric tensor, it is only possible to maintain (1) throughout the whole structure by choosing a time step less than minimum stable value:

$$\Delta t = \frac{\Delta h}{v_{\max}}, \tag{2}$$

where $v_{\max} = c/n_{\min}$ is the maximum phase velocity at a point with lowest refractive index $n_{\min}$. Now, the wave propagates less than one spatial cell during one time step and therefore, the numerical wave-length is shorter than that which would occur in continuous space. This means that spectral data generated by FDTD simulations will be shifted to longer wavelengths. This shift can be removed by choosing Δh that adequately resolves the structure. In practice, Δh is chosen first and then Δt is determined according to (2). However, smaller Δh means that more time steps are necessary to reach steady state. The Figure 1 illustrates increasing number of time steps for the 5CB liquid crystal cell with strong anchoring at both substrates and applied voltage exceeding the Freedericksz transition threshold. The refractive indexes for the 5CB are $n_0 = 1.54, n_e = 1.73$, the width of the cell is $d = 5\,\mu\text{m}$, and the wavelength of the incident light is $\lambda = 0.5\,\mu\text{m}$. The structure is embedded in glass and reflected and transmitted fields are measured inside glass with index $n = 1.54$. Polarisation of the incident light is parallel to the plane of incidence. The computation has been carried out for three different spatial resolutions: $\Delta h = \frac{\lambda}{N}, N = 20$, 40, 60. One can see that number of time steps is inversely proportional to N. So, the steady state for $N = 20$ is reached after about 1900 time steps, the steady state for $N = 40$ is reached after about 4000 time steps and 6000 time steps is required for $N = 60$. Therefore, the finer grid we choose, the longer we need to run the simulations.

COMPARISON OF FDTD METHOD RESULTS WITH ANALYTICAL METHODS

Figures (2–3) illustrate comparison of spectral data generated by FDTD method with those generated by the matrix method. Figure 2 shows the transmittance T versus λ for normal light incidence for different grid resolutions. Figure 3 shows transmittance T with $\lambda = 0.5\,\mu\text{m}$ for different angles of incidence. Transmittance in all cases was measured inside the glass.

As we expect, the FDTD data are shifted to longer wave-length and this shift is removed with increasing N. The maximum absolute errors ε

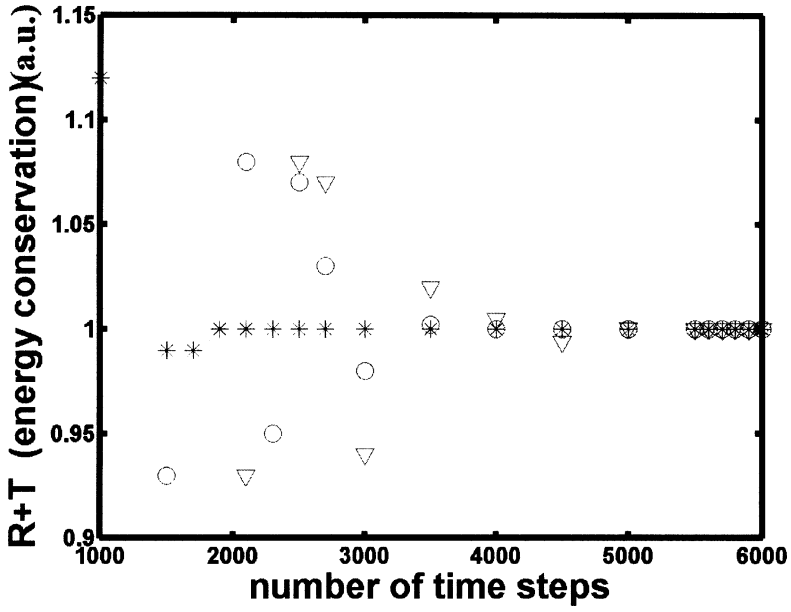

FIGURE 1

for different N are: $\varepsilon_1 = 12.5\%$ $(N = 20)$, $\varepsilon_2 = 3.4\%$ $(N = 40)$, $\varepsilon_3 = 1.2\%$ $(N = 60)$. One can see that reducing the node spacing by one-half reduces the error to one-fourth and reducing the node spacing by one-third reduces the error to 1/10. In other words, $\varepsilon \sim \Delta h^2$, which reflects the second order accuracy nature of central finite difference formula employed in FDTD method. Therefore, without resorting to higher order finite differences, improving the spatial resolution is the only way to achieve accurate FDTD results. Obviously, FDTD simulations will be more accurate for slower variation of the dielectric tensor inside the liquid crystal structure. If the spatial variation of the dielectric tensor increases, finer grids will be required for accurate results. We can see that the resolution $N = 40$ is a good compromise between time of simulation and accuracy for the considered problem, though $N =$ 60–80 may be necessary for devices containing defects such as disclinations.

TIME-RESPONSE OF LIGHT CALCULATED BY FDTD METHOD

Let us consider the planar liquid crystal structure described in the previous paragraph but with photosensitive polymer (PVK) at one of the substrates. The system is illustrated in Figure 4.

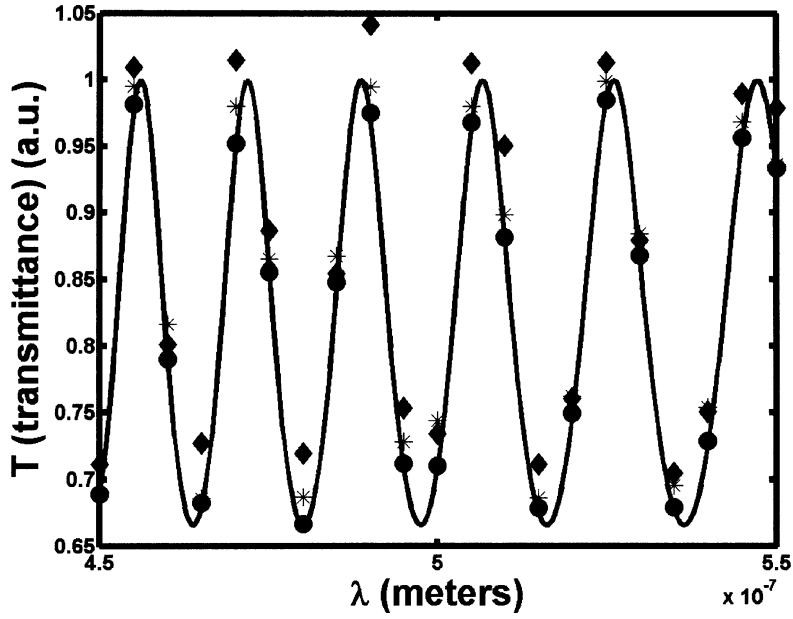

FIGURE 2

The conductivity of the polymer layer depends on the incident light. In the absence of light the conductivity is equal to zero. Therefore, when the applied voltage exceeds the Freedericksz threshold for the system without photosensitive polymer, transition does not occur because the polymer layer acts as an insulator. Once we apply an optical field to the cell, the conductivity of the polymer increases and we observe the Freedericksz transition under the applied voltage. The relaxation time for voltage $V = 10$ V is about $\tau \sim 10^{-4}$ s. During this time transmittance through the cell changes until the process of orientation finishes. Our aim is to follow these changes.

Optical wave propagation within the liquid crystal is described by Maxwell equations [7]:

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}, \tag{3}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{4}$$

$$\mathbf{D} = \varepsilon E, B = \mu_0 \mathbf{H} \tag{5}$$

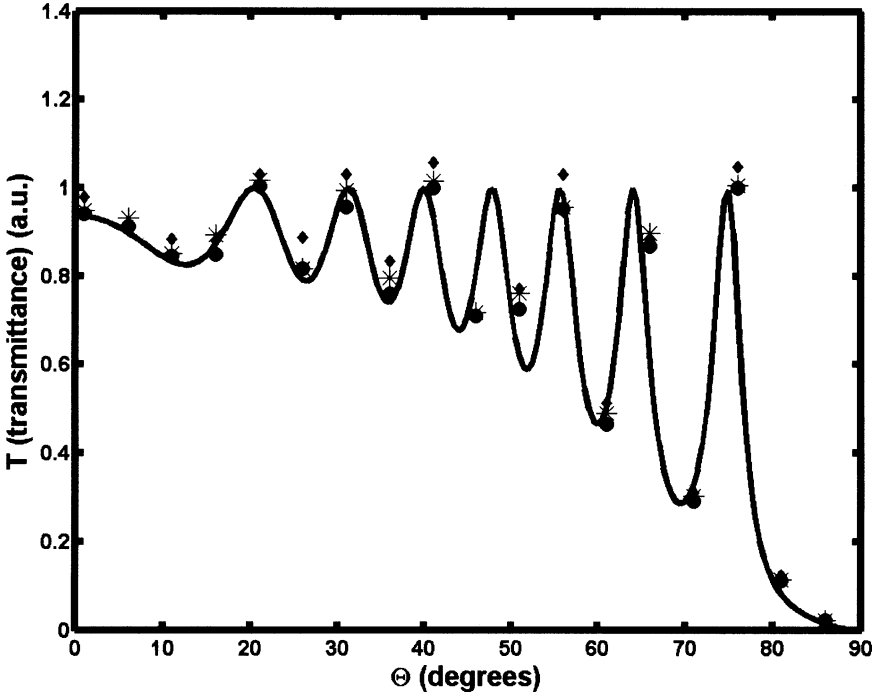

FIGURE 3

where $\tilde{\varepsilon}$ is the dielectric tensor describing the anisotropy of the liquid crystal. This tensor depends on the local director and, therefore, on the coordinate. During reorientation it also depends on time. For the described system the tensor is:

$$\tilde{\varepsilon}(z,t) = \varepsilon_0 \begin{bmatrix} n_e^2 \sin^2\theta(z,t) + n_0^2 \cos^2\theta(z,t) & 0 & (n_e^2 - n_0^2)\sin\theta(z,t)\cos\theta(z,t) \\ 0 & n_0^2 & 0 \\ (n_e^2 - n_0^2)\sin\theta(z,t)\cos\theta(z,t) & 0 & n_e^2\cos^2\theta(z,t) + n_0^2\sin^2\theta(z,t) \end{bmatrix} \tag{6}$$

Thus, changes in the director distribution will lead to changes in the solutions to Eqs. (3)–(4).

Director distribution and, therefore, $\theta(z,t)$ at each time step can be easily found from well-known equation for Freedericksz transition in an electric field [8]:

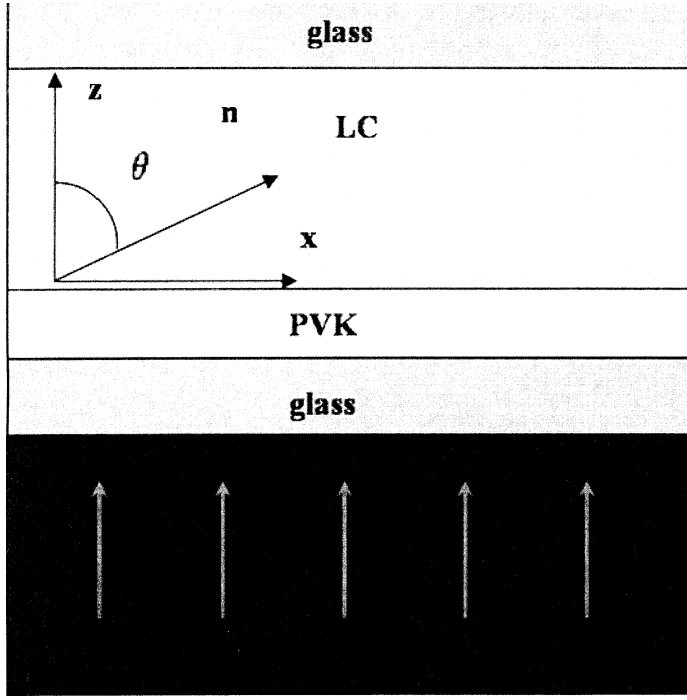

FIGURE 4

$$\gamma_1 \frac{\partial \theta(z,t)}{\partial t} = K \frac{\partial^2 \theta(z,t)}{\partial z^2} + \alpha E^2 \cos\,\theta(z,t) \sin\,\theta(z,t), \tag{7}$$

where K is the common elastic constant, E is the applied constant electric field, γ_1 is the rotational viscosity, $\alpha = \varepsilon_{||} \frac{\varepsilon_{||} - \varepsilon_\perp}{\varepsilon_\perp}$ is the parameter describing the anisotropy of the medium.

To describe the changes in transmittance we follow the following algorithm:

1. Solve Maxwell's equations (3)–(4) by FDTD method until the steady state is reached (usually relaxation time is $\tau_r \sim 10^{-13}$ s).
2. Update the theta distribution using the equation (7).
3. Update the dielectric tensor (6) and solve (3)–(4) with new director distribution.
4. Repeat until the process of reorientation is finished (relaxation time for $V = 10$ V is $\tau_r \sim 10^{-4}$ s).

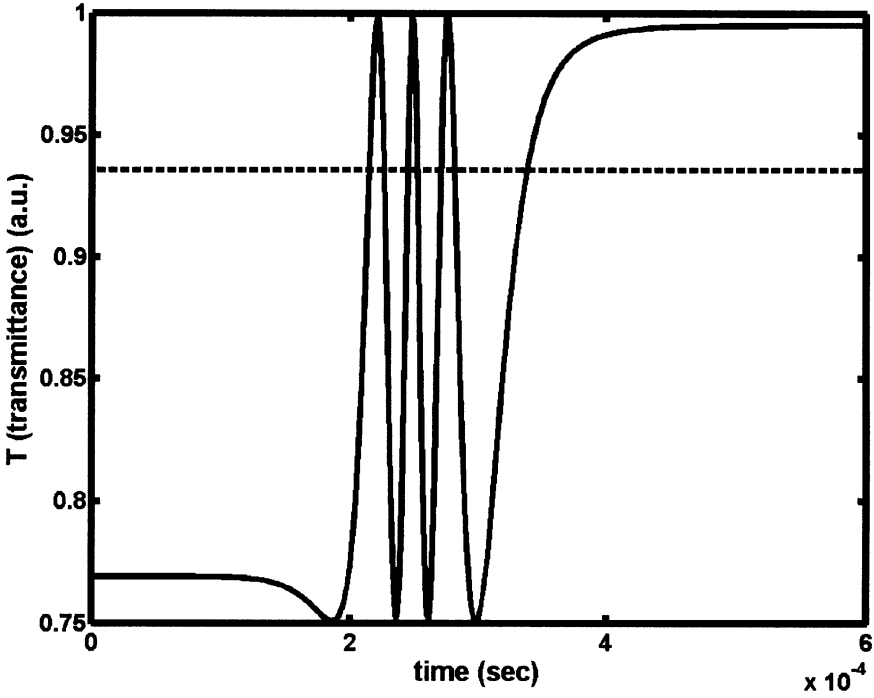

FIGURE 5

Figures (5–6) illustrate changes in light transmittance with time. Transmittance for normal incidence is shown in Figure 5. The black line describes the change of parallel polarisation that coincides in this case with extraordinary wave. It experiences refractive index in x-z plane. As reorientation happens in this plane, the index changes its value starting from the extraordinary index n_e at $t = 0$. Because of this, the wave changes its phase many times before the end of reorientation and we observe change of transmittance. Finally by $t = 6^*10^{-4}$ sec it reached equilibrium.

Red line describes perpendicular polarisation. This polarisation experiences refractive index in y-z plane. This index does not change and coincides with ordinary index n_0 of liquid crystal. Therefore, transmittance of this polarisation is not affected.

Figure 6 shows the results for a 45 degrees angle of incidence. Again, the transmittance of perpendicular polarisation does not change because the wave still remains in the y-z plane. Transmittance of extraordinary wave exhibits similar behaviour to the previous case.

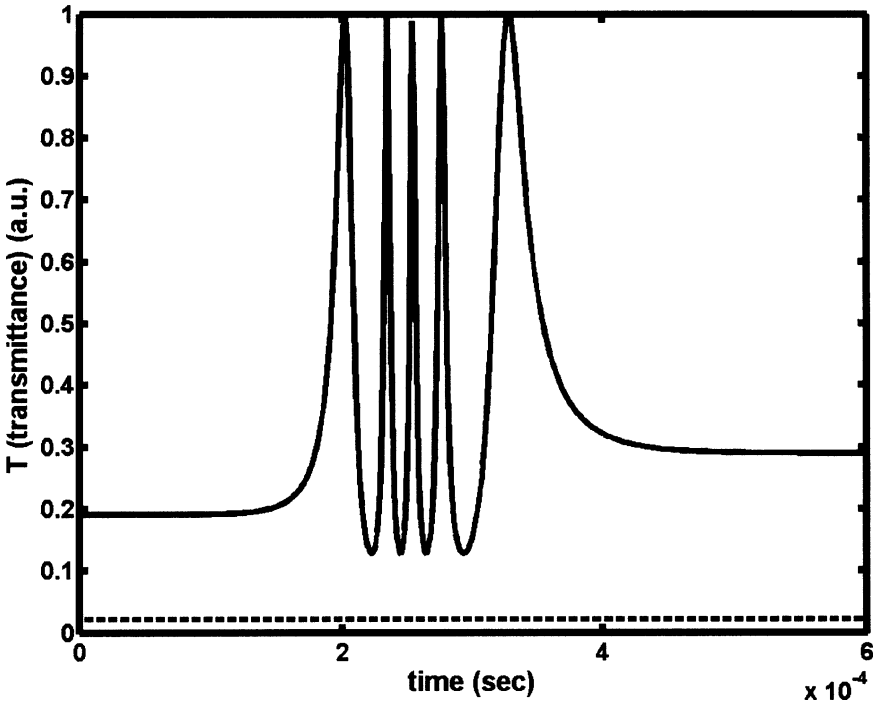

FIGURE 6

CONCLUSIONS

In this paper we have compared FDTD method results with analytical method results for a nematic liquid crystal cell with an applied voltage for different wavelengths and angles of incidence of light. Analysis suggests that attention must be paid to choosing the spatial discretisation as the error decreases for finer grids. The choice would depend on the spatial rate of change of the refractive index of the medium: more rapid variation of the refractive index requires a finer grid for accurate modelling.

We have also introduced an algorithm for solving the time dependent problem where we can take into account changes in propagation due to changes in the director distribution. The considered problem is one dimensional but nevertheless provides insight into the usage of the FDTD method for liquid crystal structures. The future work includes extension of the algorithm to two dimensions and dealing with non linear phenomena where time response analysis is required, such as interference and diffraction effects.

REFERENCES

[1] Berreman, D. W. (1972). *J. Opt. Soc. Am.*, *62*, 502.
[2] Lien, A. (1990). *Appl. Phys. Lett.*, *57*, 2767.
[3] Taflove, A. (1995). Computational Electrodynamics: The Finite-Difference Time-Domain Method, Artech House, Boston.
[4] Titus, C. M., Bos, P. J., Kelly, J. R., & Gartland, E. C. (1999). *Jpn. J. Appl. Phys.*, *Part 1*, *38*, 1488.
[5] Yee, K. S. (1966). *IEEE Trans. Ant. Prop.*, *AP-14*, 302.
[6] Berenger, J. -P. (1994). *J. Comp. Phys.*, *114*, 185.
[7] Amnon, Y. (1984). *Optical Waves in Crystals : Propagation and Control of Laser Radiation*, New York: Wiley.
[8] Priestley, E. B., Peter J. Wojtowicz, & Ping Sheng (Eds.). (1975). Introduction to liquid crystals, Plenum Press: New York.