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## Liquid Crystals

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# Optical wave propagation in a cholesteric liquid crystal using the finite element method

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Bragg reflections of cholesteric liquid crystals at normal and oblique incidences were investigated using the finite element method (FEM). Detailed FEM derivations together with the consideration of boundary conditions are given. Two methods for achieving broadband Bragg reflection are analysed: one is to use high birefringence liquid crystal in the uniform pitch structure, the other is to use the gradient pitch structure. In each case, the number of cholesteric pitches required for establishing the Bragg reflection was simulated.

## 1. Introduction

A broadband cholesteric liquid crystal (Ch-LC) has important applications for reflective displays and diffusive reflectors and reflective polarizers [1–3]. The Ch-LC cell is typically prepared by doping some chiral agents into a nematic LC mixture. Such cholesteric structure is periodic around a preferred axis and the spatial period is equal to half of the pitch length  $P_0$ . The Bragg reflection of the incident light occurs around the central wavelength  $\lambda_0 = nP_0$ . Only the incident light with the same circular polarization as the cholesteric helix is strongly reflected, and the opposite circular polarization is transmitted without any significant reflection. This scattering depends on the birefringence and the chiral arrangement of the rod-shape molecules [1–9].

To analyse the light propagation in the cholesteric medium, the  $4 \times 4$  matrix method has been developed [10]. The  $4 \times 4$  matrix method is fast, however it is difficult to be used to solve two-dimensional and three-dimensional problems, especially when the geometry is complex. In this paper, we investigate the Bragg reflection properties of cholesteric LCs using the finite element method (FEM). FEM is a well recognized numerical method since a general purpose computer program can be easily developed to analyse rigorously the problems where analytical solutions are difficult to

obtain, e.g. the three-dimensional modelling of liquid crystal devices. Moreover, FEM has the advantages of easy convergence in the space domain, and unconditional convergence and high order error in the time domain, as compared with the finite difference time domain (FDTD) method [11–14], which is another well recognized numerical method in optical simulations. Moreover, the parameter matrices of the differential equation are sparse in the finite element method. If we take the advantage of sparse matrix, the calculation time can be reduced significantly.

To broaden the reflection bandwidth, the high birefringence and gradient pitch methods are commonly used. We apply our finite element method to analyse the reflection bandwidths of these two modes at normal and oblique incidences.

## 2. Numerical modelling

### 2.1. Finite element formulations

For the cholesteric LC, there is a spiral structure of the liquid crystal directors as shown in figure 1. This chiral structure has a periodicity  $P_0$ , which is known as the pitch length. In this case, the dielectric tensor is only a function of the  $z$ -coordinate as given by [1]:

$$\varepsilon(z) = \begin{bmatrix} \varepsilon_{11}(z) & \varepsilon_{12}(z) & \varepsilon_{13}(z) \\ \varepsilon_{21}(z) & \varepsilon_{22}(z) & \varepsilon_{23}(z) \\ \varepsilon_{31}(z) & \varepsilon_{32}(z) & \varepsilon_{33}(z) \end{bmatrix} \quad (1)$$

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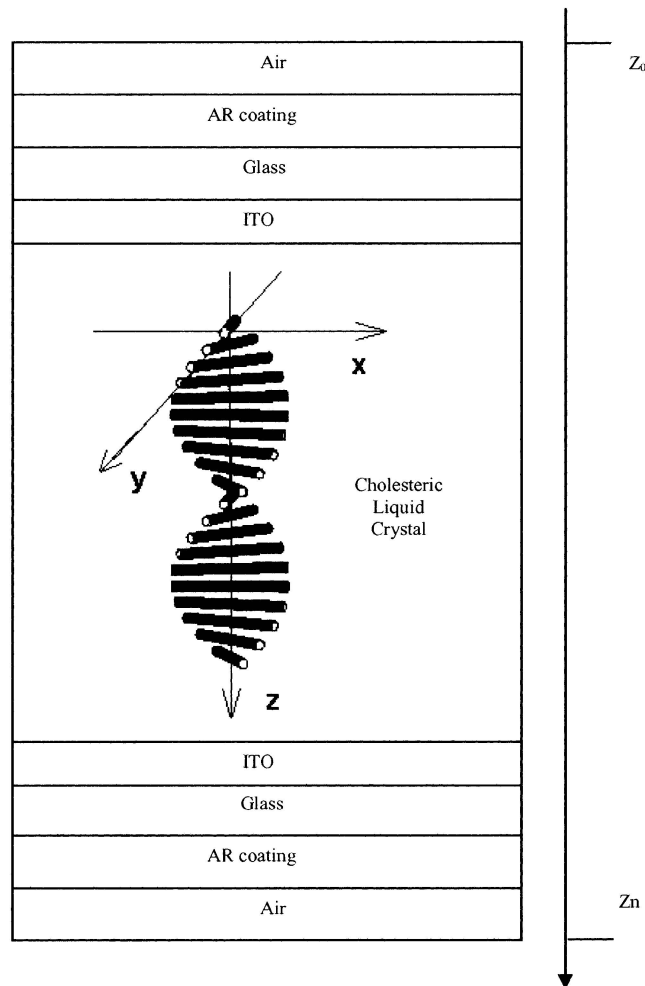


Figure 1. The cholesteric structure used for simulations.

where

$$\varepsilon_{11}(z) = \frac{1}{2}(\varepsilon_{\parallel} + \varepsilon_{\perp}) + \frac{1}{2}(\varepsilon_{\parallel} - \varepsilon_{\perp}) \cos\left(\frac{4\pi}{P_0}z\right)$$

$$\varepsilon_{22}(z) = \frac{1}{2}(\varepsilon_{\parallel} + \varepsilon_{\perp}) - \frac{1}{2}(\varepsilon_{\parallel} - \varepsilon_{\perp}) \cos\left(\frac{4\pi}{P_0}z\right)$$

$$\varepsilon_{12}(z) = \frac{1}{2}(\varepsilon_{\parallel} - \varepsilon_{\perp}) \sin\left(\frac{4\pi}{P_0}z\right)$$

$$\varepsilon_{21}(z) = \varepsilon_{12}(z)$$

$$\varepsilon_{33}(z) = \varepsilon_{\perp}.$$

Here  $P_0$ ,  $\varepsilon_{\parallel}$  and  $\varepsilon_{\perp}$  are the cholesteric pitch length, and the dielectric constants perpendicular and parallel to the liquid crystal director, respectively.

In a special case when  $\varepsilon_{13}$ ,  $\varepsilon_{23}$ ,  $\varepsilon_{31}$  and  $\varepsilon_{32}$  are equal to zero, the following equations can be derived from

Maxwell's equations [1]:

$$\frac{\partial}{\partial z} \begin{bmatrix} E_x \\ E_y \\ H_x \\ H_y \end{bmatrix} = jk_0 \begin{bmatrix} 0 & 0 & 0 & \eta_0 \left( \frac{k_x^2}{k_0^2} \frac{1}{\varepsilon_{33}} - 1 \right) \\ 0 & 0 & \eta_0 & 0 \\ \frac{\varepsilon_{21}}{\eta_0} & \frac{1}{\eta_0} \left( \varepsilon_{22} - \frac{k_x^2}{k_0^2} \right) & 0 & 0 \\ -\frac{\varepsilon_{11}}{\eta_0} & -\frac{\varepsilon_{12}}{\eta_0} & 0 & 0 \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ H_x \\ H_y \end{bmatrix} \quad (2)$$

$$\times \begin{bmatrix} E_x \\ E_y \\ H_x \\ H_y \end{bmatrix} = jk_0 \begin{bmatrix} 0 & \eta_0 \underline{Q}_H \\ \frac{1}{\eta_0} \underline{Q}_E & 0 \end{bmatrix} \cdot \begin{bmatrix} E_x \\ E_y \\ H_x \\ H_y \end{bmatrix}$$

where

$$k_x = k_0 \sin \theta \quad \text{and} \quad \eta_0 = \sqrt{\mu_0/\varepsilon_0}$$

$$\underline{Q}_E = \begin{bmatrix} \varepsilon_{21} & \left( \varepsilon_{22} - \frac{k_x^2}{k_0^2} \right) \\ -\varepsilon_{11} & -\varepsilon_{12} \end{bmatrix}$$

$$\underline{Q}_H = \begin{bmatrix} 0 & \left( \frac{k_x^2}{k_0^2} \frac{1}{\varepsilon_{33}} - 1 \right) \\ 1 & 0 \end{bmatrix}.$$

From equation (2), we can derive the following one-dimensional wave equations for  $E_x$  and  $E_y$  as

$$\frac{d}{dz} \left( \frac{1}{k_0} \underline{Q}_H^{-1} \frac{d}{dz} \begin{bmatrix} E_x \\ E_y \end{bmatrix} \right) + k_0 \underline{Q}_E \begin{bmatrix} E_x \\ E_y \end{bmatrix} = 0. \quad (3)$$

Using the Galerkin method [12] to solve the wave equations, equation (3) is expressed in the weak form as:

$$\int_{z_0}^{z_n} \left[ \left( -\frac{1}{k_0} \underline{Q}_H^{-1} \right) \frac{dW_n}{dz} \cdot \frac{d}{dz} \begin{bmatrix} E_x \\ E_y \end{bmatrix} + k_0 \underline{Q}_E W_n \begin{bmatrix} E_x \\ E_y \end{bmatrix} \right] dz + \frac{1}{k_0} \underline{Q}_H^{-1} W_n \frac{d}{dz} \begin{bmatrix} E_x \\ E_y \end{bmatrix} \Big|_{z=z_0}^{z=z_n} = 0 \quad (4)$$

where  $W_n$  is the weighting function.

Applying the finite element method, in the  $z$ -direction, the liquid crystal region is discretized by a second order uniform mesh as shown in figure 2. The electric field



where the entries of matrix  $[A]$  are given by:

$$A_{ij}^e = \int_{z_i^e}^{z_j^e} \left[ \left( -\frac{1}{k_0} \underline{\underline{Q}}_H^{-1} \right) \frac{dN_i^e(z)}{dz} \cdot \frac{dN_j^e(z)}{dz} + k_0 \underline{\underline{Q}}_E N_i^e(z) N_j^e(z) \right] dz.$$

Solving equation (10) will give the electric field intensity along the  $z$ -direction.

### 2.2. Absorbing boundary condition

We can apply the absorbing boundary condition to the transmitted and reflected waves. For the perpendicularly polarized incident wave as shown in figure 2, the total wave at the boundary of both  $z = z_0$  and  $z = z_n$  is

$$\mathbf{E} = \mathbf{E}^i + \mathbf{E}^r \quad (11)$$

where the incident wave is

$$\mathbf{E}^i = \exp(-jk_z z) \cdot \mathbf{a}_y,$$

and the reflected wave is

$$\mathbf{E}^r = \Gamma \exp(jk_z z) \cdot \mathbf{a}_y.$$

From equation (11), the reflected wave at the boundary  $z = z_0$  is:

$$\mathbf{E}^r = \mathbf{E} - \mathbf{E}^i. \quad (12)$$

If we take the differentiation of  $\mathbf{E}^r$  with respect to  $z$ , we have  $\partial/\partial z \mathbf{E}^r = jk_z \mathbf{E}^r$ . Hence, by differentiating both sides of equation (11) with respect to  $z$ , we can obtain:

$$\frac{\partial}{\partial z} (\mathbf{E} - \mathbf{E}^i) - jk_z (\mathbf{E} - \mathbf{E}^r) = 0$$

from which we get:

$$\frac{\partial}{\partial z} E_y \Big|_{z=z_0} - jk_z E_y|_{z=z_0} = -2jk_z E_y^i|_{z=z_0}. \quad (13)$$

At the boundary  $z = z_n$ , since there is no reflection, the total wave is:

$$\mathbf{E} = \mathbf{E}^t. \quad (14)$$

Using the same procedure as discussed before, we have:

$$\frac{\partial}{\partial z} E_y \Big|_{z=z_n} + jk_z E_y|_{z=z_n} = 0. \quad (15)$$

Likewise, we find the absorbing boundary condition of the parallel polarized incident wave as:

$$\frac{\partial}{\partial z} E_x \Big|_{z=z_0} - jk_z E_x|_{z=z_0} = -2jk_z E_x^i|_{z=z_0} \quad (16)$$

$$\frac{\partial}{\partial z} E_x \Big|_{z=z_n} + jk_z E_x|_{z=z_n} = 0.$$

The circularly polarized wave can be composed from the linearly polarized waves as:

$$\begin{aligned} \mathbf{E}_{\text{RCP}} &= (E_x \mathbf{a}_x + jE_y \mathbf{a}_y)/2 \\ \mathbf{E}_{\text{LCP}} &= (E_x \mathbf{a}_x - jE_y \mathbf{a}_y)/2. \end{aligned} \quad (17)$$

### 2.3. Reflectance and transmittance

After solving the wave equations, the reflected and the transmitted waves can be obtained from equations (12) and (14), respectively. Hence, the reflectance of the TE, TM, LCP (left-hand circular polarization) and RCP waves at the boundary  $z = z_0$  can be solved as

$$\begin{aligned} \Gamma_{\text{TE}} &= E_y^r / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \\ \Gamma_{\text{TM}} &= (E_x^r / \cos \theta)^2 / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \\ \Gamma_{\text{LCP}} &= (E_x^r / \cos \theta + jE_y^r)^2 / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \\ \Gamma_{\text{RCP}} &= (E_x^r / \cos \theta - jE_y^r)^2 / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \end{aligned} \quad (18)$$

where  $\theta$  is the oblique incident angle.

The transmittance of TE, TM, LCP and RCP wave at the boundary  $z = z_n$  can be found as

$$\begin{aligned} T_{\text{TE}} &= E_y^t / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \\ T_{\text{TM}} &= (E_x^t / \cos \theta)^2 / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \\ T_{\text{LCP}} &= (E_x^t / \cos \theta + jE_y^t)^2 / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \\ T_{\text{RCP}} &= (E_x^t / \cos \theta - jE_y^t)^2 / [(E_x^i / \cos \theta)^2 + E_y^i{}^2] \end{aligned} \quad (19)$$

### 2.4. Glass and AR coating layers

Reflection at the interface of air and LC occurs due to their dielectric constant difference. To minimize this reflection and make the simulation more realistic, both sides of the glass substrates are coated with six-layer anti-reflection (AR) films, as shown in figure 1. The AR coating films are designed with Binomial Transformer [12]. The dielectric constants  $\varepsilon_{\perp}$  and  $\varepsilon_{\parallel}$  are equal to each other inside the glass and AR coating layers so that equations (1) to (8) are still valid through the whole solution region.

## 3. Simulation results and discussions

### 3.1. Comparison between the FEM and the $4 \times 4$ -matrix method

To validate the accuracy of the FEM model, we compare its results with those obtained by the  $4 \times 4$  matrix method. The simulated Bragg reflection spectra using the  $4 \times 4$  matrix method and the finite element method for the case of normal incidence are shown in figure 3(a). The same comparison for the  $20^\circ$  oblique angle incidence inside the liquid crystal media is shown in figure 3(b). For both methods, Bragg reflection spans about 60 nm bandwidth, centred at  $\lambda_0 = 550$  nm for the normal incidence,

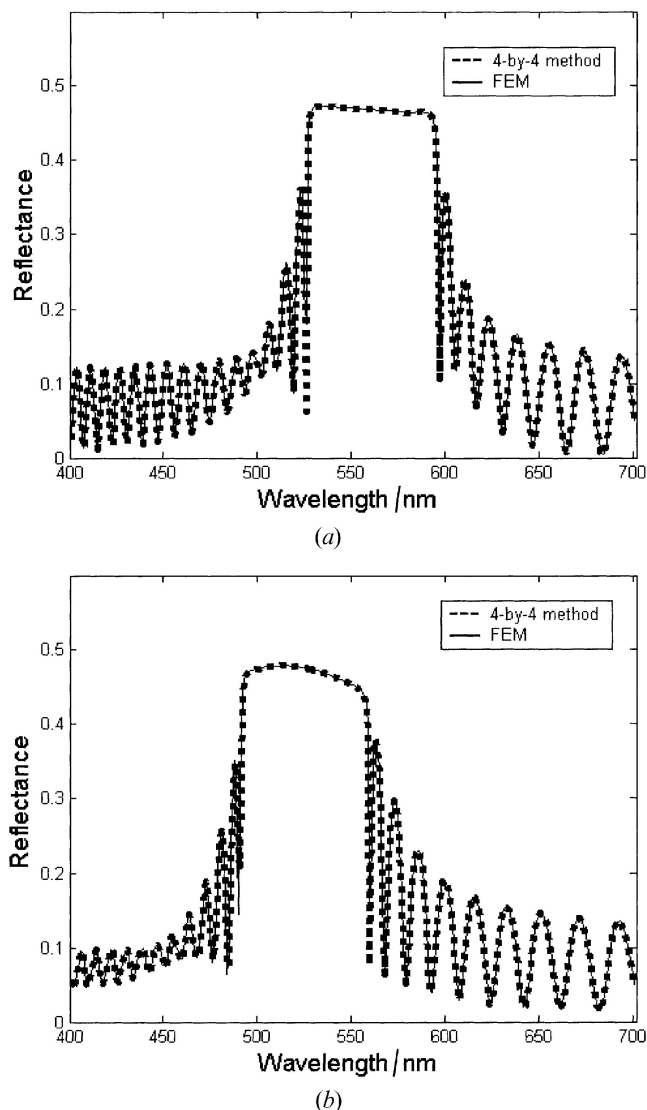


Figure 3. Comparison of Bragg reflection between the finite element method and the  $4 \times 4$  matrix method: (a) normal incidence; (b) oblique incidence at  $20^\circ$  inside the LC layer. Ch-LC:  $P_0 = 329$  nm,  $\Delta n = 0.2$  and  $n_e = 1.8$ . The FEM results overlap almost perfectly with those obtained from the  $4 \times 4$  matrix method.

and centred at 525 nm for the  $20^\circ$  oblique incidence. In both simulations, the reflections from glass and LC interfaces are ignored. Our FEM results overlap perfectly with those obtained from the  $4 \times 4$  method. The two results are almost indistinguishable.

### 3.2. Central wavelength of Bragg reflection

At the normal incidence, the helical pitches of the cholesteric LC layers introduce the Bragg reflection centred at wavelength  $\lambda_0$  [1]:

$$\lambda_0 = nP_0 \quad (20)$$

where  $P_0$  is the pitch length of the cholesteric liquid crystal and  $n$  is the average refractive index defined by [15–17]:

$$n^2 = (n_e^2 + 2n_o^2)/3. \quad (21)$$

For an oblique incidence wave propagating at an angle of  $\theta$  inside the liquid crystal, the central wavelength of Bragg reflection is governed by:

$$\lambda = nP_0 \cos \theta \quad (22)$$

where  $\theta$  can be obtained by Snell's law as:

$$\theta = \sin^{-1} \left( \frac{1}{n} \sin \theta \right). \quad (23)$$

The relationship between the angle  $\theta$  and the central wavelength of Bragg reflection is responsible for the blue shift [1, 4, 8].

### 3.3. Broadband Bragg reflection

Broadband Bragg reflection is highly desirable for electronic books and reflective polarizers as it will broaden the bandwidth and therefore enhance the display brightness. Another important application is that it will compensate for the blue shift shown in figure 4 if the bandwidth is sufficiently wide. The bandwidth of Bragg reflection is given by

$$\Delta\lambda = \Delta n P_0 \quad (24)$$

where  $\Delta n = n_e - n_o$  is the birefringence of the liquid crystal. To expand the Bragg reflection to cover the entire visible region, two approaches are often considered. A straightforward method is to use a high birefringence LC.

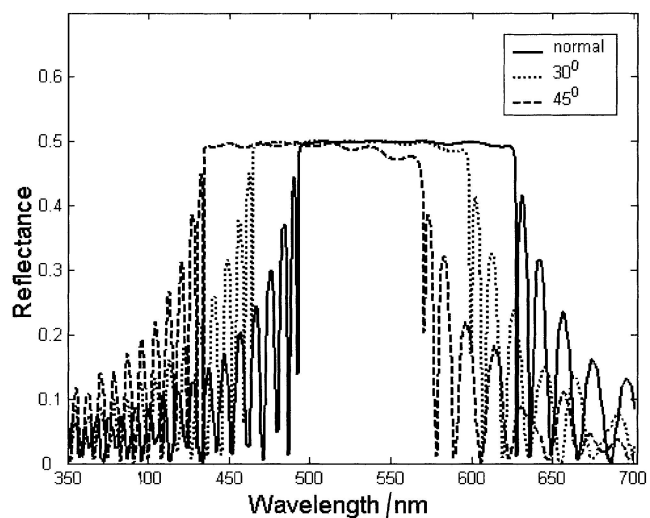


Figure 4. Blue shift on the Bragg reflection of a right-handed cholesteric LC. Ch-LC cell:  $P_0 = 330$  nm,  $d = 16P_0$ ,  $\Delta n = 0.4$  and  $n_o = 1.5$ . The glass substrates and AR coating layers are included in the calculations.

Two cholesteric liquid crystal materials with birefringence of 0.2 and 0.6 are compared in figure 5. The LC with  $\Delta n \sim 0.2$  shows a 75 nm bandwidth. If the LC  $\Delta n$  is increased to 0.6, the reflection bandwidth is increased to  $\sim 200$  nm. As the material research advances, LC compounds with  $\Delta n > 0.5$  have been developed [1]. In these simulations, the LC cell gap is fixed at  $16 P_0$ . The pitch length in each simulation is chosen so that the central wavelength of the Bragg reflection occurs at 550 nm.

An alternative approach to broaden reflection bandwidth is to use cholesteric liquid crystals with gradient pitch length. Figure 6 compares simulated results with pitch linearly varying from 240 to 350 nm (solid lines) and uniform pitch (dashed lines;  $P_0 = 310$  nm). In the former case, the bandwidth covers from 450 to 800 nm for the  $\Delta n \sim 0.4$  LC employed. For the uniform pitch cell, the bandwidth (from 510 to 640 nm) is much narrower. However, in the gradient pitch approach, the interference of the liquid crystal chiral structure on the optical wave is not strong enough to establish Bragg reflection in the first few pitches. As a result, a thicker LC layer is needed. The drawback of a thick LC layer is its increased operating voltage.

In the gradient pitch approach, we have compared the linear and exponential pitch profiles. We assume the pitch grows from 240 to 350 nm within the cell gap. The gradients of the increased pitch length are given by:

$$\begin{aligned} P_{\text{linear}} &= P_0 \cdot (1 + 0.458z/d) \\ P_{\text{exp}} &= P_0 \exp(0.377z/d) \end{aligned} \quad (25)$$

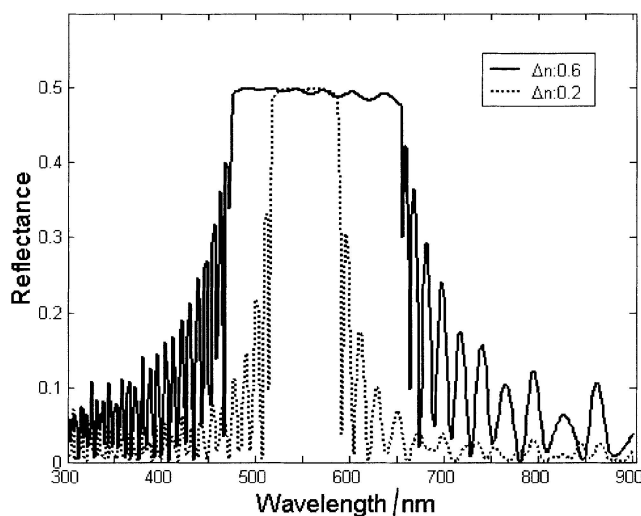


Figure 5. Bragg reflections of the right-hand cholesteric LCs with different birefringence at normal incidence. Ch-LC: uniform pitch length and  $d = 16P_0$ . The  $\Delta n$  of the LC materials is 0.2 and 0.6, and their ordinary refractive index is assumed to be 1.5 and 1.6, respectively. The pitch length in each simulation is set so that the central wavelength of the Bragg reflection is 550 nm.

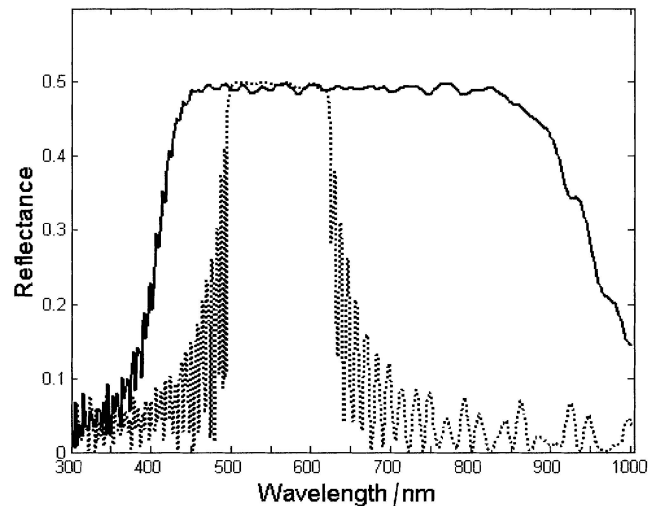


Figure 6. Bragg reflections of the right-hand Ch-LCs with uniform (dashed lines) and linearly increased (solid lines) pitch length. In both simulations,  $\Delta n = 0.4$ ,  $n_o = 1.6$ ,  $d = 24P_0$  and  $P_0 = 310$  nm. For the Ch-LC with linearly gradient pitch,  $P_0$  increases from 240 to 350 nm as described in equation (25).

In equation (25),  $z$  and  $d$  are the direction coordinate and the LC cell gap, respectively, and  $P_0 = 240$  nm. The simulation results are shown in figure 7. The cholesteric liquid crystal with exponentially increased pitch length profile provides somewhat wider bandwidth than the linearly increased case. However, the bandwidth of the peak Bragg reflection is rather similar; both cover from 420 to 900 nm.

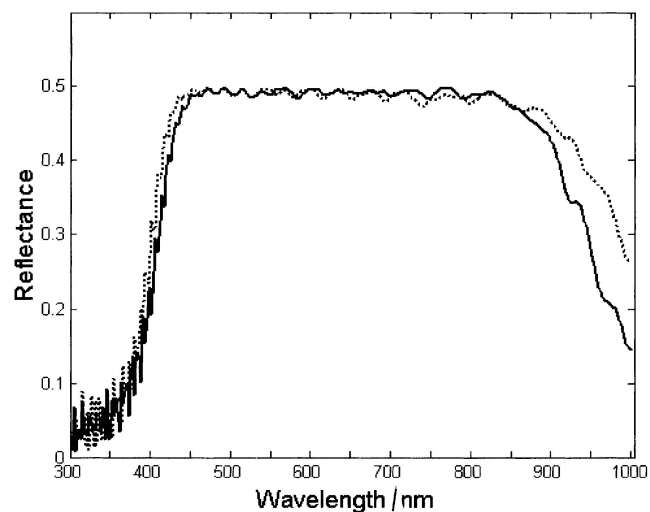


Figure 7. Comparison of Bragg reflections between Ch-LC with linearly (solid lines) and exponentially (dashed lines) increased pitch length. LC:  $\Delta n = 0.4$  and  $n_o = 1.6$ ,  $d = 24P_0$  and  $P_0 = 240$  nm. In both cases, the pitch length increases from 240 to 350 nm as described in equation (25).

From figure 7, the gradient pitch length technology dramatically increases the reflection bandwidth as compared with the traditional uniform pitch length approach. Thus, this method allows lower birefringence LC materials to be used for achieving a black and white Ch-LCD. The exponential pitch profile has been realized by UV treatment of the cholesteric LC sample containing photocurable monomer [18, 19].

### 3.4. Establishment of Bragg reflection

The strongly constructive interference of the reflected light inside the helical molecular structure is responsible for the observed Bragg reflection. In order to establish the Bragg reflection, a minimum cholesteric layer thickness is needed [1]. We have analysed such transient phenomena using FEM, and the simulation results are depicted in figure 8. For the uniform pitch cholesteric LC, Bragg reflection is established when the film thickness is larger than  $10P_0$ , where  $P_0$  is the pitch length.

For a cholesteric liquid crystal with gradient pitch length, the pitch length is increased along the optical wave propagating direction. A thicker film is required in order to have sufficient pitches to establish the Bragg reflection. Figures 9 and 10 show the simulation results for the linear and exponential pitch profiles, respectively. In each case, an LC layer of more than  $20P_0$  thickness is required for establishing the Bragg reflection. The required thickness of the liquid crystal film depends on the expected Bragg reflection spectrum and the pitch length profile. For a given LC mixture, a thicker cholesteric film would result in a higher operating voltage.

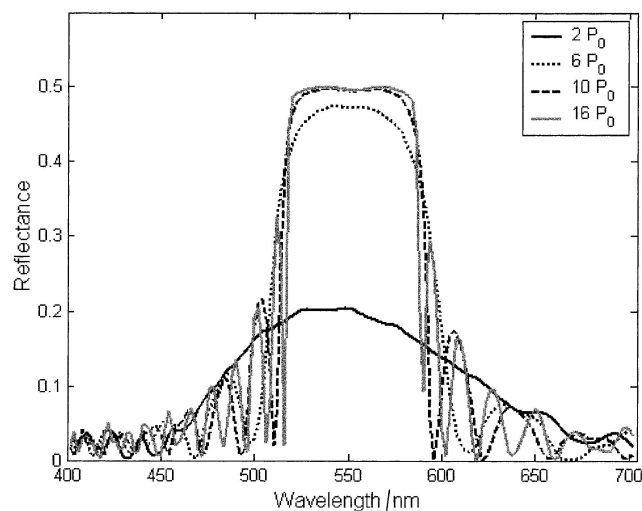


Figure 8. The establishment of Bragg reflection for a Ch-LC film with uniform pitch length at normal incidence. LC:  $\Delta n = 0.4$ ,  $n_o = 1.6$  and  $P_0 = 310$  nm.

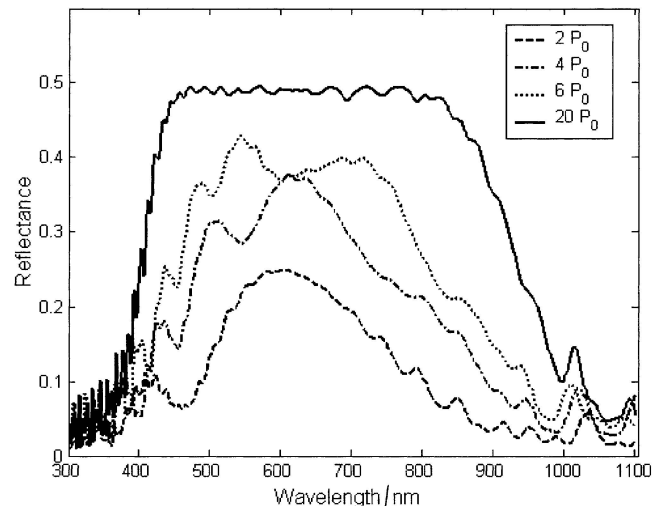


Figure 9. The establishment of Bragg reflection for a Ch-LC film with linearly increased pitch length at normal incidence. LC:  $\Delta n = 0.4$ ,  $n_o = 1.6$  and  $P_0$  increases linearly from 240 to 350 nm as described in equation (25).

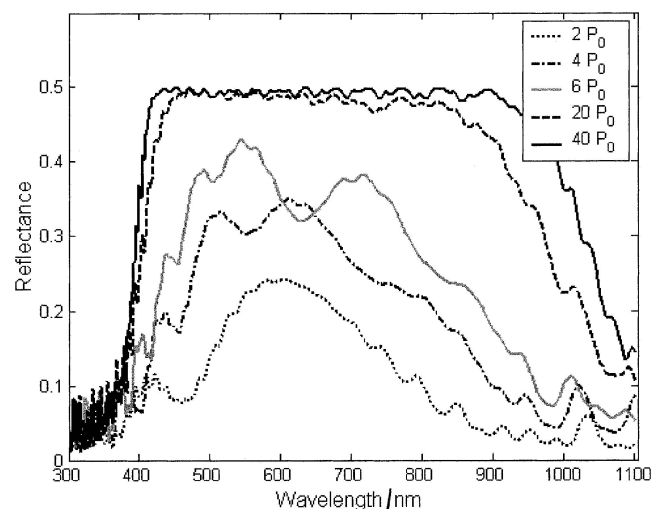


Figure 10. The establishment of Bragg reflection for a Ch-LC film with exponentially increased pitch length at normal incidence. LC:  $\Delta n = 0.4$ ,  $n_o = 1.6$ , and  $P_0$  increases from 240 to 350 nm exponentially as described in equation (25).

The results shown in figures 8–10 are for normal incidence. In oblique angle incidence, there is a strong coupling between the left-hand and right-hand circularly polarized waves when the wavelength reaches the Mauguin limit [1, 4, 8], as shown in figure 11. The profile of gradient pitch length enhances the coupling because of the short pitch length at the first few pitches. Furthermore, if the film is thicker the polarization coupling will be stronger, since there are more short pitch layers. When designing a cholesteric liquid crystal



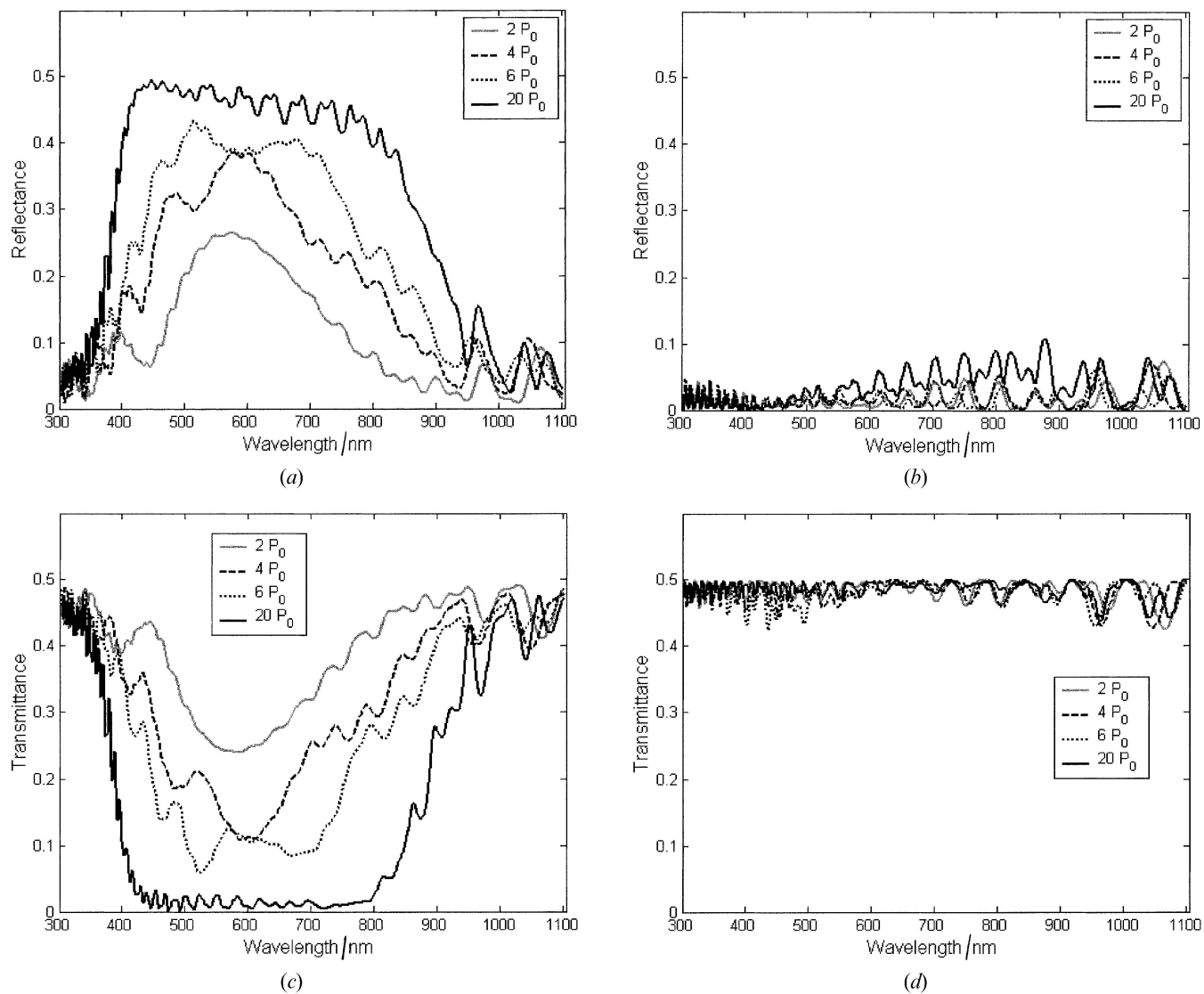


Figure 11. Polarization coupling of Bragg reflection for the Ch-LC with linearly increased pitch length at  $30^\circ$  viewing angle: (a) reflectance of the RCP wave; (b) reflectance of the LCP wave; (c) transmittance of the RCP wave; (d) transmittance of the LCP wave. LC:  $\Delta n = 0.4$ ,  $n_o = 1.6$  and  $P_0$  increases linearly from 240 to 350 nm.

device, the balance between Bragg reflection bandwidth, film thickness, and polarization coupling in oblique angle incidence all need to be taken into consideration.

#### 4. Conclusions

We have developed the finite element method for investigating the Bragg reflections of cholesteric liquid crystals. One-dimensional modelling of a cholesteric liquid crystal using the finite element method has been introduced. Two approaches for achieving broadband Bragg reflection have been analysed. The method of using a uniform pitch and high birefringence LC has the advantage of easy fabrication except that the required  $\Delta n$  is quite high. The gradient pitch method dramatically increases the bandwidth of Bragg reflection while the

birefringence is relative smaller. Furthermore, the required LC film thickness has been investigated for the establishment of Bragg reflection as well as the polarization coupling of the oblique incidence waves.

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