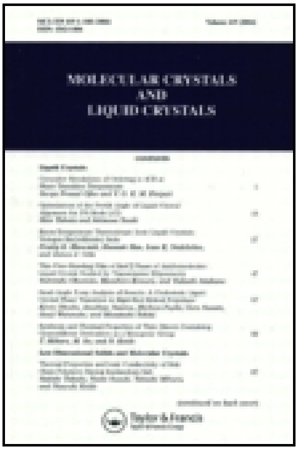

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Optics in Stratified Media—The Use of Optical Eigenmodes of Uniaxial Crystals in the 4 × 4-Matrix Formalism

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A new method of evaluating the optical properties of stratified uniaxial media is proposed. Within Berreman's 4 × 4 matrix formalism, the exact propagator of a homogeneous layer is used instead of the Taylor series expansion. The calculation of the transmission and reflection matrices for a given propagator is performed. Examples are given to demonstrate the usefulness of the proposed method.

INTRODUCTION

Since the invention of twisted nematic liquid-crystal displays (TN LCD's) in 1971,[1] great progress has been made in designing suitable liquid-crystal materials (LC) and display manufacturing processes. There were developed several new types of LCD's which perform the increasing requirements of application branches. With the ever increasing demands for large area flat panel displays, a good understanding and optimization of the optical performance of LCD's is desired.

The most commonly used nematic or chiral nematic LC's are optically uniaxial anisotropic media. Therefore the design of these LCD's splits into two steps: First, one has to compute the spatial arrangement of the local optical axis (called the director configuration) by means of the continuum theory[2] and then the optical performance can be computed. The LCD is usually assumed to represent a stratified medium, i.e., the direction of the local optical axis (director) varies only in one direction perpendicular to the boundary plates.

Several matrix techniques were developed by Jones,[3] Teitler and Henvis[4] and Berreman and Scheffer[5–8] to solve the problem of reflection and transmission in stratified media, the most clear and general being that of Berreman and Scheffer. Their 4 × 4-matrix method is often used in the literature.[9]

Except for the case of a few analytical solutions, this method requires numerical computations. In a medium where the dielectric tensor varies with position computations can be performed by breaking the medium up into a series of thin layers with a nearly constant dielectric tensor. Each layer can then be treated as a homogeneous anisotropic medium. Berreman and Scheffer wrote the characteristic matrix of such a layer as a series expansion in powers of its thickness, which is assumed to be a small parameter so that terms with high powers could be ignored.[7] Actually this approximation and the convergence of the series requires very thin layers, even if the layer is actually homogeneous.

Another method was reported by Abdulhalim *et al.*[10] who found an exact solution for a homogeneous layer using the Sylvester-Lagrange interpolation polynomial.

In our work we will show how the well-known optical eigenmodes (OEM) of a homogeneous uniaxial crystal can be used to calculate thet exact characteristic matrix of a homogeneous layer. This method is much faster than the reported solutions, because the thickness of the layers can be chosen dependent only on the variation of the optical axis.

THEORY

Consider a stratified, locally uniaxial medium whose optical axis varies only in the z-direction. The 4×4-matrix method consists of computing a 4×4-matrix, P, called the propagator, of complex numbers that depend on the dielectric and other optical parameters of the medium, its thickness, and the propagation vector of the incident light[7] which is assumed to be a plane wave, such that

$$\Phi(d) = P\,\Phi(0) \qquad \text{where } \Phi(z) = \begin{bmatrix} \sqrt{\epsilon_0} & E_x(z) \\ \sqrt{\mu_0} & H_y(z) \\ \sqrt{\epsilon_0} & E_y(z) \\ -\sqrt{\mu_0} & H_x(z) \end{bmatrix} \tag{1}$$

where d is the thickness of the planar structure, E and H are the electric and magnetic field components parallel to the surfaces, and ϵ_0 and μ_0 are the dielectric and magnetic vacuum constants, respectively. The light is incident in the xz-plane.

It can be seen, that the propagator for a thick sample is equal to the matrix product of P's for any complete series of subintervals between 0 and d.

The differential form of the same equation may be written as[7]

$$d\Phi/dz = ik_0\,\Delta\Phi \tag{2}$$

with $k_0 = \Omega/c$, where Ω is the angular frequency of the incident light and c is its vacuum velocity; Δ is a 4×4 matrix. The matrix P is found by integrating Equation (2), giving

$$P(d) = R\,\exp(ik_0 \int_0^d \Delta(z)dz)$$

Here the operator R defines the ordering of the $\Delta(z)$ matrices in the expansion of the exponential in analogy to Dyson's time ordering operator T in quantum electrodynamics.

As we already mentioned the propagator of a stratified sample can be computed by matrix multiplication of the characteristic matrices of homogeneous layers. Therefore we consider now the case of a homogeneous uniaxial medium, i.e., the matrix Δ in Equation (2) does not depend on z. In this case the solution can be symbolically written as

$$P = \exp(ik_0\,\Delta h) \tag{3}$$

where h is the sample thickness. In order to compute P exactly we have to diagonalize the matrix Δ.

The matrix Δ of a non-magnetic medium with dielectric tensor ϵ is given by

$$\Delta = \begin{bmatrix} -\varkappa_x \dfrac{\epsilon_{zx}}{\epsilon_{zz}} & 1 - \dfrac{\varkappa_x^2}{\epsilon_{zz}} & -\varkappa_x \dfrac{\epsilon_{zy}}{\epsilon_{zz}} & 0 \\ \epsilon_{xx} - \dfrac{\epsilon_{xz}\epsilon_{zx}}{\epsilon_{zz}} & -\varkappa_x \dfrac{\epsilon_{xz}}{\epsilon_{zz}} & \epsilon_{xy} - \dfrac{\epsilon_{xz}\epsilon_{zy}}{\epsilon_{zz}} & 0 \\ 0 & 0 & 0 & 1 \\ \epsilon_{yx} - \dfrac{\epsilon_{yz}\epsilon_{zx}}{\epsilon_{zz}} & -\varkappa_x \dfrac{\epsilon_{yz}}{\epsilon_{zz}} & \epsilon_{yy} - \dfrac{\epsilon_{yz}\epsilon_{zy}}{\epsilon_{zz}} - \varkappa_x^2 & 0 \end{bmatrix} \tag{4}$$

Here $\varkappa_x$ denotes the x-component of the "refractive index vector" which is defined by

$$\boldsymbol{\varkappa} = \frac{\mathbf{k}}{k_0} = (\varkappa_x, 0, \varkappa_z) \tag{5}$$

where $\mathbf{k}$ is the wave vector of the incident planar wave. As we assume the light is incident in the xz-plane, the y-component of $\boldsymbol{\varkappa}$ vanishes. According to the stratification in z-direction, $\varkappa_x$ is a constant through the sample.

Let $\mathbf{n}$ be a unit vector in the direction of the optical axis of the crystal (called the director). The dielectric tensor is given by

$$\epsilon_{\alpha\beta} = \epsilon_\perp\,\delta_{\alpha\beta} + \Delta\epsilon n_\alpha n_\beta \tag{6}$$

Here α,β stands for x,y,z and $\epsilon_\|,\epsilon_\perp$ are the dielectric constants perpendicular and parallel to the director, respectively. $\Delta\epsilon$ is called the anisotropy of the dielectric tensor, $\delta_{\alpha\beta}$ denotes the Kronecker symbol and n_α are the components of $\mathbf{n}$.

In order to diagonalize Δ we compute the OEM as solutions of the equation

$$\Delta\Phi = \varkappa_z\Phi \tag{7}$$

This leads first to the secular equation

$$|\Delta - \varkappa_z I| = 0 \tag{8}$$

where $|\cdot \cdot \cdot|$ denotes the determinant, $\varkappa_z$ the eigenvalue and I the identity matrix. The fourth order equation (8) for the eigenvalue can be explicitly written as a product of two quadratic terms:

$$(\epsilon_\perp - \varkappa_x^2 - \varkappa_z^2)(\epsilon_\parallel\epsilon_\perp - \epsilon_\perp\varkappa_x^2 - \epsilon_\perp\varkappa_z^2 - \Delta\epsilon[\varkappa_x n_x + \varkappa_z n_z]^2) = 0 \tag{9}$$

This equation can easily be solved and we get two classes of eigenvalues

$$\varkappa_{zo\pm} = \pm\sqrt{\epsilon_\perp - \varkappa_x^2} \tag{10}$$

$$\varkappa_{ze\pm} = -\varkappa_x \frac{\epsilon_{xz}}{\epsilon_{zz}} \pm \sqrt{\frac{\epsilon_\parallel\epsilon_\perp}{\epsilon_{zz}} - \varkappa_x^2 \cdot \frac{\epsilon_{xx}\epsilon_{zz} - \epsilon_{xz}^2}{\epsilon_{zz}^2}} \tag{11}$$

with the corresponding eigenvectors $\Phi_{o\pm}$ and $\Phi_{e\pm}$ given by

$$\Phi_{o\pm} = \begin{bmatrix} -n_y\varkappa_{zo\pm} \\ -\epsilon_\perp n_y \\ n_x\varkappa_{zo\pm} - n_z\varkappa_x \\ \varkappa_{zo\pm}[n_x\varkappa_{zo\pm} - n_z\varkappa_x] \end{bmatrix} \quad \Phi_{e\pm} = \begin{bmatrix} n_x - \frac{\varkappa_x}{\epsilon_\perp}(n_x\varkappa_x + n_z\varkappa_{ze\pm}) \\ n_x\varkappa_{ze\pm} - n_z\varkappa_x \\ n_y \\ n_y\varkappa_{ze\pm} \end{bmatrix} \begin{matrix}(12)\\(13)\end{matrix}$$

The eigenvectors represent the well-known ordinary and extraordinary waves in a uniaxial crystal denoted by the indices *o* and *e* respectively. The electrical field of the ordinary wave is polarized perpendicular to the plane in which the director and the propagation vector lie, whilst the magnetic field of the extraordinary wave is perpendicular to this plane.

If we combine the OEM as column vectors to a matrix T with

$$T = (\Phi_{e+}, \Phi_{e-}, \Phi_{o+}, \Phi_{o-}) \tag{14}$$

we see immediately that Equation (7) leads to

$$\Delta T = T \begin{pmatrix} \varkappa_{ze+} & & & 0 \\ & \varkappa_{ze-} & & \\ & & \varkappa_{zo+} & \\ 0 & & & \varkappa_{zo-} \end{pmatrix} \tag{15}$$

Hence it follows from Equations (3) and (15)

$$P = T N T^{-1} \tag{16}$$

where

$$N = \begin{pmatrix} \exp(ik_o h\varkappa_{ze+}) & & & 0 \\ & \exp(ik_o h\varkappa_{ze-}) & & \\ & & \exp(ik_o h\varkappa_{zo+}) & \\ 0 & & & \exp(ik_o h\varkappa_{zo-}) \end{pmatrix} \tag{17}$$

The problem now is to find the inverse of the matrix T. This can be done by using a special condition for non-absorbing media, which are characterized by a real, symmetric dielectric tensor. As one can see by straightforward calculation using Equation (4) the following condition holds:

$$\Sigma_x \Delta = \Delta^+ \Sigma_x \tag{18}$$

where

$$\Sigma_x = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

We consider now two OEM Φ_m, Φ_k to the eigenvalues $\varkappa_m, \varkappa_k$. Then

$$\frac{d}{dz}\{\Phi_m^+ \Sigma_x \Phi_k\} = \frac{d\Phi_m^+}{dz}\Sigma_x \Phi_k + \Phi_m^+ \Sigma_x \frac{d\Phi_k}{dz}$$

$$= ik_0 \Phi_m^+ (\Delta^+ \Sigma_x - \Sigma_x \Delta)\Phi_k = 0$$

On the other hand

$$\Delta \Phi_k = \varkappa_k \Phi_k \qquad \Phi_m^+ \Delta^+ = \Phi_m^+ \varkappa_m^*$$

Hence it follows

$$(\varkappa_k - \varkappa_m^*)\Phi_m^+ \Sigma_x \Phi_k = 0 \tag{19}$$

Φ^+ denotes the conjugated complex and transposed vector to Φ. Equation (19) is called "Potier's relation"[11] and represents a generalized orthogonality of the OEM.[12] It is a consequence of the conservation of energy in the z-direction.

Using Equation (19) we get the following relation for the matrix T:

$$T^+ \Sigma_x T = S \equiv \begin{pmatrix} S_{e+e+} & S_{e+e-} & & 0 \\ S_{e-e+} & S_{e-e-} & & \\ & & S_{o+o+} & S_{o+o-} \\ 0 & & S_{o-o+} & S_{o-o-} \end{pmatrix} \tag{20}$$

A straightforward calculation leads to the elements of S:

$$S_{o\pm o\pm} = \begin{cases} 2\varkappa_{zo\pm}\,[\epsilon_\perp(1 - n_z^2) + \varkappa_x^2(n_z^2 - n_x^2) - 2n_xn_z\varkappa_x\varkappa_{zo\pm}] \text{ for } \varkappa^*_{zo\pm} = \varkappa_{zo\pm} \\ 0 \text{ for } \varkappa^*_{zo\pm} = -\varkappa_{zo\pm} \end{cases} \tag{21}$$

$$S_{o\pm o\mp} = \begin{cases} 0 \text{ for } \varkappa^*_{zo\pm} = \varkappa_{zo\pm} \\ 2\varkappa_{zo\mp}[\epsilon_\perp(1 - n_z^2) + \varkappa_x^2(n_z^2 - n_x^2) - 2n_xn_z\varkappa_x\varkappa_{zo\mp}] \text{ for } \varkappa^*_{zo\pm} = -\varkappa_{zo\pm} \end{cases}$$

$$S_{e\pm e\pm} = \begin{cases} 2[\varkappa_{ze\pm}(1 - n_z^2 + \frac{\varkappa_x^2}{\epsilon_\perp}[n_z^2 - n_x^2]) + \frac{\varkappa_x}{\epsilon_\perp} n_xn_z\,(\varkappa_x^2 - \epsilon_\perp - \varkappa_{ze\pm}^2)] \\ \quad \text{for } \varkappa^*_{ze\pm} = \varkappa_{ze\pm} \\ 0 \text{ for } \varkappa^*_{ze\pm} \neq \varkappa_{ze\pm} \end{cases}$$

$$S_{e\pm e\mp} = \begin{cases} 0 \text{ for } \varkappa^*_{ze\pm} = \varkappa_{ze\pm} \\ 2[\varkappa_{ze\mp}(1 - n_z^2 + \frac{\varkappa_x^2}{\epsilon_\perp}[n_z^2 - n_x^2]) + \frac{\varkappa_x}{\epsilon_\perp} n_xn_z(\varkappa_x^2 - \epsilon_\perp - \varkappa_{ze\mp}^2)] \\ \quad \text{for } \varkappa^*_{ze\pm} \neq \varkappa_{ze\pm} \end{cases}$$

Now we see that

$$S^{-1}T^+\,\Sigma_xT = I \tag{22}$$

and hence

$$T^{-1} = S^{-1}T^+\Sigma_x \tag{23}$$

The inversion of S is very easy to compute and we get as the final result for the propagator

$$P = T\,N\,S^{-1}T^+\Sigma_x \tag{24}$$

Note that the method only works if the eigenvalues are different from each other. The singular cases with equal eigenvalues can be obtained by taking the limes of Equation (24) or by another method which will be reported later.

REFLECTION AND TRANSMISSION

For a given propagator P of the stratified medium we shall now calculate reflection and transmission coefficients of the medium between two isotropic media. We consider the electrical field components of the incident, reflected and transmitted light (see Figure 1).

As shown in Figure 1, $A_\parallel$, $A_\perp$ denote the electrical field components in the plane of incidence and perpendicular to it. The same definitions are used for the reflected

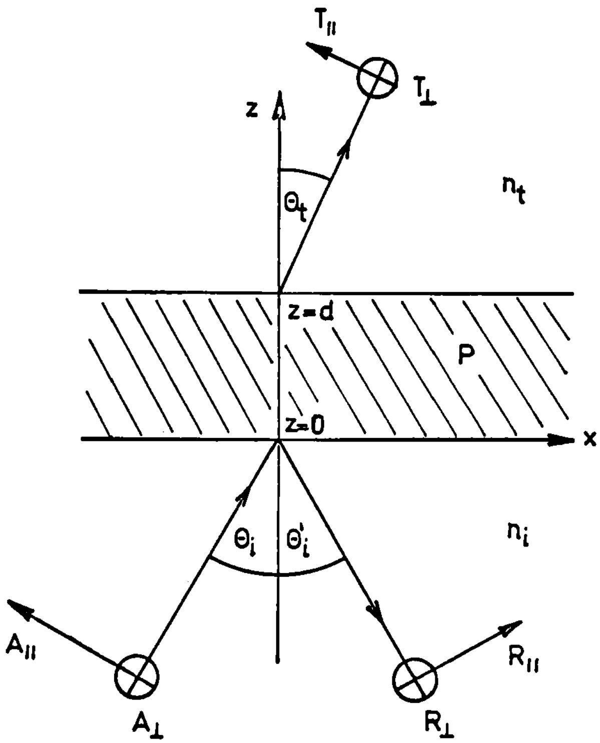

FIGURE 1 Definition of the directions of the electrical field components in the plane of incidence and perpendicular to it.

($R_{\parallel}$, $R_{\perp}$) and the transmitted light ($T_{\parallel}$, $T_{\perp}$). The angle θ_i to the z-axis is the angle of incidence of the light which is equal to the reflection angle θ_i'. The angle θ_t between the transmitted light and the z-direction can be calculated by Snell's law:

$$\cos\theta_t = [1 - (n_i \sin\theta_i / n_t)^2]^{1/2} \tag{25}$$

where n_i and n_t are the corresponding refractive indices. Using these definitions we can describe the propagation vectors $\Phi(0)$ and $\Phi(d)$ in terms of a new vector $\tilde{\psi}(0)$ and $\tilde{\psi}(d)$ which contains only the electrical field components:

$$\tilde{\psi}(0) = \sqrt{\epsilon_0}\begin{pmatrix} A_{\parallel} \\ R_{\parallel} \\ A_{\perp} \\ R_{\perp} \end{pmatrix} \qquad \tilde{\psi}(d) = \sqrt{\epsilon_0}\begin{pmatrix} T_{\parallel} \\ 0 \\ T_{\perp} \\ 0 \end{pmatrix} \tag{26}$$

The relation between Φ and $\tilde{\psi}$ is obtained using Maxwell's equations in the isotropic media.

$$\text{with} \qquad \Phi(z) = U(z)\tilde{\psi}(z) \qquad z = 0,d \tag{27}$$

$$U(z) = \begin{pmatrix} -\cos\theta_\alpha & \cos\theta_\alpha & & 0 \\ -n_\alpha & -n_\alpha & & \\ & & 1 & 1 \\ & 0 & n_\alpha\cos\theta_\alpha & -n_\alpha\cos\theta_\alpha \end{pmatrix} \qquad \begin{array}{l} z = 0,d \\ \alpha = i,t \end{array} \tag{28}$$

From Equation (27) we obtain

$$\tilde{\psi}(d) = Q\tilde{\psi}(0) \qquad \text{with } Q = U^{-1}(d)\,PU(0) \tag{29}$$

This equation may be written explicitly as:

$$\begin{pmatrix} T_\parallel \\ T_\perp \end{pmatrix} = \begin{pmatrix} Q_{11} & Q_{13} \\ Q_{31} & Q_{33} \end{pmatrix}\begin{pmatrix} A_\parallel \\ A_\perp \end{pmatrix} + \begin{pmatrix} Q_{12} & Q_{14} \\ Q_{22} & Q_{24} \end{pmatrix}\begin{pmatrix} R_\parallel \\ R_\perp \end{pmatrix} \tag{30}$$

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} Q_{21} & Q_{23} \\ Q_{41} & Q_{43} \end{pmatrix}\begin{pmatrix} A_\parallel \\ A_\perp \end{pmatrix} + \begin{pmatrix} Q_{22} & Q_{24} \\ Q_{42} & Q_{44} \end{pmatrix}\begin{pmatrix} R_\parallel \\ R_\perp \end{pmatrix} \tag{31}$$

(The Q_{ij} denote the matrix elements of Q in the i-th row and j-th column.)

We define the reflection and transmission matrices r and t by:

$$\begin{pmatrix} T_\parallel \\ T_\perp \end{pmatrix} = t\begin{pmatrix} A_\parallel \\ A_\perp \end{pmatrix} \qquad \begin{pmatrix} R_\parallel \\ R_\perp \end{pmatrix} = r\begin{pmatrix} A_\parallel \\ A_\perp \end{pmatrix} \tag{32}$$

And we can compute r and t using Equations (30) and (31):

$$r = -\begin{pmatrix} Q_{22} & Q_{24} \\ Q_{42} & Q_{44} \end{pmatrix}^{-1}\begin{pmatrix} Q_{21} & Q_{23} \\ Q_{41} & Q_{43} \end{pmatrix} \tag{33}$$

$$t = \begin{pmatrix} Q_{11} & Q_{13} \\ Q_{31} & Q_{33} \end{pmatrix} + \begin{pmatrix} Q_{12} & Q_{14} \\ Q_{22} & Q_{24} \end{pmatrix} r \tag{34}$$

The 2×2-matrices r and t describe the influence of the medium characterized by the propagator P on the electrical field components. The corresponding intensity ratios are the squares of the absolute values of the matrix elements and will be denoted by

$$R_{\alpha\beta} = |r_{\alpha\beta}|^2 \qquad T_{\alpha\beta} = |t_{\alpha\beta}|^2 \qquad (\alpha,\beta = p \text{ or } s) \tag{35}$$

EXAMPLES

In order to demonstrate the formalism described in the previous section we have calculated transmission TSS curves for the selective reflection in chiral smectic C phases with the following parameter set: $n_e = 1.6$; $n_o = 1.4$; tilt angle $\theta = 30°$;

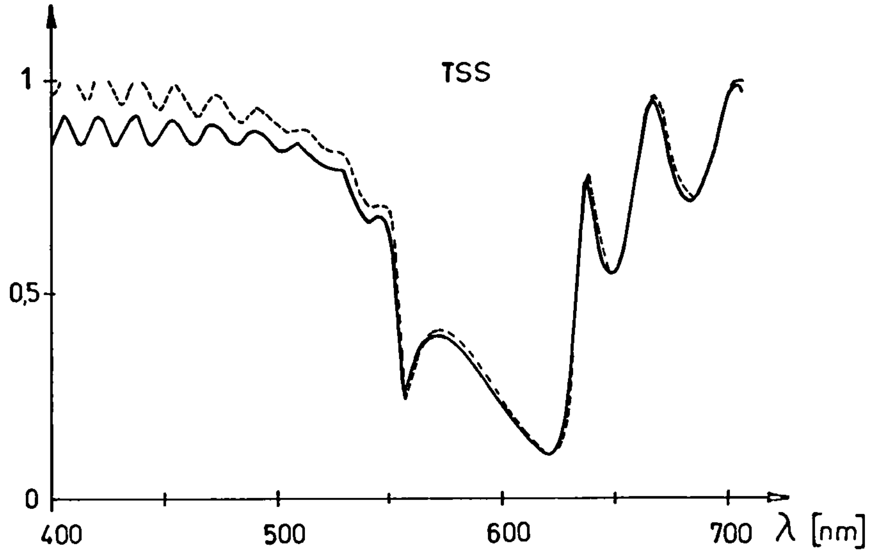

FIGURE 2 Transmission TSS *versus* wavelength curves for light propagation along the helix axis in a chiral smectic C using the OEM method (solid line) and the Taylor series expansion (broken line). The parameters are given in the text.

pitch $p = 0.4$ μm and cell thickness $d = 4$ μm. Figure 2 shows the dependence of the transmission TSS on the wavelength for the case of normal incidence, i.e., for light propagation along the helix axis. For the computation, the cell has been divided into 500 layers. In this case the result obtained by the use of the OEM (solid line) corresponds to the exact solution for a smectic C*.[13] The result for TSS by use of the Taylor expansion up to the second order in each layer is given by

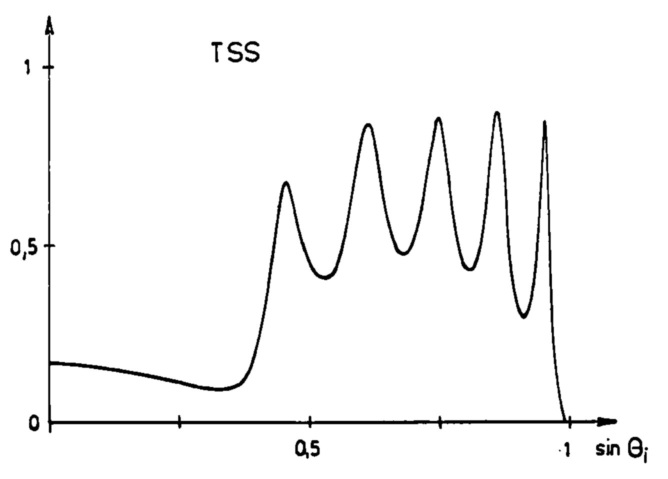

FIGURE 3 Dependence of the transmission TSS on the angle of incidence θ_i for a wavelength of 600 nm.

the broken line in Figure 2. As can be seen, the TSS values obtained from the Taylor expansion differ significantly from the exact solution for wavelengths below the selective reflection band. It has already been mentioned by Berreman,[7] that a good convergence of the series method can be achieved either by using a higher order expansion or more layers. The second order expansion always converges if enough layers are used.[7] For example, the agreement of the second order expansion with the reported OEM method in Figure 2 is very good if the number of layers is doubled. This demonstrates the advantage of our proposed OEM method, which gives higher accuracy of the results with less computational effort. Figure 3 shows the dependence of the transmission TSS on the angle of incidence θ_i for the same parameters and a wavelength of 600 nm inside the selective reflection band. The Bragg reflections are clearly visible giving a further proof of the usefulness of the applied method.

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