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Approximate Scalar Finite-Element Analysis of Anisotropic Optical Waveguides with Off-Diagonal Elements in a Permittivity Tensor

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Abstract — An approximate scalar finite-element program for the analysis of anisotropic optical waveguides having a permittivity tensor with nonzero off-diagonal elements is described. In this approach, the nonphysical spurious solutions which are included in the solutions of the earlier vectorial finite-element method in an axial-components formulation do not appear. Numerical examples on an anisotropic dielectric rectangular waveguide composed of a uniaxial medium are given. Our results for the waveguide whose optic axis lies in the plane (xy-plane) normal to the direction (z-axis) of propagation agree well with the results of the vectorial wave analysis using the variational method. We also demonstrate the application of this approach by analyzing the anisotropic dielectric rectangular waveguide whose optic axis lies in the xz- or yz-plane.

I. INTRODUCTION

Several methods for the analysis of a three-dimensional optical waveguide such as shown in Fig. 1 (where \( t \) is the height or depth and \( W \) is the width) have been proposed [1] and the vectorial finite-element method in an axial components \((E_z - H_z)\) formulation, which enables one to compute accurately the mode spectrum of a waveguide with arbitrary cross section, is widely used [2]–[8]. However, the vectorial finite-element solutions have been known to include nonphysical solutions [2]–[8]. If one wants to compute a set of eigenmodes, it is difficult and very cumbersome to distinguish between the spurious and the physical modes of the guides. The cause of these spurious modes is believed to be in the indefinite nature of the \( E_z - H_z \) variational formulation [6]–[8]. In addition, the vectorial finite-element method can be applied only to anisotropic waveguides with a diagonal permittivity tensor [3], [7].

Recently, Steinberg and Giallorenzi [9] have formulated an approximate coupled mode treatment based on the Marcatili method [10] for a uniaxial waveguide whose optic axis lies in the xz-plane, and Ohtaka [11] has analyzed a uniaxial waveguide whose optic axis lies in the xy-plane using the variational method. Mabaya, Lagasse, and Vandenberghe [7] have presented an approximate scalar finite-element formulation for the analysis of isotropic optical waveguides. This approach has as its main advantages: the smaller matrix dimensions, less computer time, no spurious modes (because functionals based on the scalar approximation are positive definite [7]), and the capability of easily computing higher order modes [7], [12], [13].

In this paper, this approximate scalar finite-element method is extended to the anisotropic waveguides having a permittivity tensor with nonzero off-diagonal elements. For two-dimensional waveguides \((\partial / \partial x = 0)\) [14]–[17], the matrix equation derived by this approach is reduced to the exact expression for two-dimensional guided modes [18], [19]. In order to study the accuracy of the method, various isotropic dielectric waveguides are analyzed and the results obtained are compared with previously published results [5], [10], [20]. Then, numerical examples on an anisotropic dielectric rectangular waveguide composed of a uniaxial medium are given. Our results for the waveguide whose optic axis lies in the xy-plane agree well with the results of the vectorial wave analysis using the variational method [11]. We also demonstrate the application of this approach by analyzing the anisotropic dielectric rectangular waveguide whose optic axis lies in the xz- or yz-plane.

Fig. 1. Three-dimensional optical waveguide geometry.

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II. APPROXIMATE BASIC EQUATIONS

We consider a three-dimensional anisotropic waveguide in Fig. 1 having a permittivity tensor with all nonzero off-diagonal elements ε_{ij}K_{ij} (i, j = x, y, z) and the permeability of free space μ₀, where ε_{0} is the permittivity of free space and K_{ij} is the relative permittivity.

Maxwell’s equations are, in component form

\[ \frac{\partial E_x}{\partial y} + jk_z E_y = -j\omega\varepsilon_0 H_x \]
\[ \frac{\partial E_y}{\partial x} - \frac{\partial E_z}{\partial y} = -j\omega\varepsilon_0 H_y \]
\[ \frac{\partial E_z}{\partial x} + jk_z H_y = j\omega\mu_0 H_z \]
\[ \frac{\partial H_x}{\partial y} + jk_z H_y = j\omega\mu_0 E_x \]
\[ \frac{\partial H_y}{\partial x} - \frac{\partial H_z}{\partial y} = j\omega\mu_0 E_y \]
\[ \frac{\partial H_z}{\partial x} + jk_z E_y = j\omega\mu_0 E_z \]

where E_{x}, H_{x}, and D_{x} are the electric field, the magnetic field, and the electric flux density, respectively, and ω and k_{z} are the angular frequency and the wavenumber in the z-direction, respectively.

The constitutive relations are

\[ D_x = \varepsilon_0 (K_{xx}E_x + K_{xy}E_y + K_{xz}E_z) \]
\[ D_y = \varepsilon_0 (K_{xy}E_x + K_{yy}E_y + K_{yz}E_z) \]
\[ D_z = \varepsilon_0 (K_{xz}E_x + K_{yz}E_y + K_{zz}E_z) \]

We assume |K_{ij}| ≪ K_{ii} (i ≠ j) and a small index variation in the lateral (x) direction, then we may approximate as

\[ K_{ij}\partial/\partial x \approx 0, \quad i \neq j. \]  \hspace{1cm} (12)

Considering (12), from (2) and (11) we obtain

\[ H_y = \frac{1}{j\omega\mu_0} \left( jk_z E_x + \frac{1}{\varepsilon_0 K_{zz}} \frac{\partial D_z}{\partial x} \right). \]  \hspace{1cm} (13)

Substituting (8) into (13) and considering (9), (10), and (12), we obtain

\[ H_y = \frac{1}{j\omega\mu_0} \left[ jk_z E_x + \frac{1}{\varepsilon_0 K_{zz}} \frac{\partial D_z}{\partial x} \right]. \]  \hspace{1cm} (14)

We write (3)

\[ H_z = \frac{1}{j\omega\mu_0} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right). \]  \hspace{1cm} (15)

Considering (10)–(12) and eliminating E_{z} between (5) and (6), we obtain

\[ E_z = \frac{1}{j\omega\varepsilon_0} \left( \frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} \right) \frac{b}{a} E_x. \]  \hspace{1cm} (16)

Substituting (7) into (16), we obtain

\[ E_y = \frac{1}{j\omega\varepsilon_0} \left[ jk_z K_{zz}H_x + \frac{K_{xz}}{jk_z} \frac{\partial H_z}{\partial x} - \frac{K_{yy}}{jk_z} \frac{\partial H_y}{\partial y} \right] \frac{b}{a} E_x. \]  \hspace{1cm} (17)

Considering (10)–(12) and eliminating E_{y} between (5) and (6), we obtain

\[ E_x = \frac{1}{j\omega\varepsilon_0} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_z}{\partial y} \right) \frac{c}{a} E_y. \]  \hspace{1cm} (18)

where

\[ a = K_{yy} K_{zz} - K_{xz}^2 \]  \hspace{1cm} (19a)
\[ b = K_{xy} K_{zz} - K_{xz} K_{yz} \]  \hspace{1cm} (19b)
\[ c = K_{xz} K_{yy} - K_{xy} K_{yz} \]  \hspace{1cm} (19c)

Substituting (14), (15), (17), and (18) into (4), considering (12) and neglecting the terms of E_{y} in the same manner as in the isotropic case [7], [12], we obtain

\[ \frac{K_{xx}}{K_{zz}} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \left( \frac{k_0^2}{a} \left( K_{xx} - K_{xy} \frac{b}{a} - K_{xz} \frac{c}{a} \right)^2 - K_{zz}^2 \right) \phi 
- k_0 k_{zz} \psi + jk_0 \frac{c}{a} \psi = 0. \]  \hspace{1cm} (20)

Similarly, substituting (17) and (18) into (1) and neglecting the terms of H_{y} in the same manner as in the isotropic case [7], [12], we obtain

\[ \frac{K_{zz}}{a} \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} \left( \frac{K_{yy}}{a} \frac{\partial \psi}{\partial y} - jk_0 K_{yzz} \psi + jk_0 \frac{c}{a} \phi \right) 
+ \left( k_0^2 - K_{zz} \frac{k_0^2}{a} \right) \psi - jk_z \frac{K_{yz}}{a} \frac{\partial \psi}{\partial y} - k_0 k_{zz} \frac{b}{a} \phi = 0. \]  \hspace{1cm} (21)

where

\[ \phi = E_x \]  \hspace{1cm} (22)
\[ \psi = \eta_0 H_x \]  \hspace{1cm} (23)
\[ k_0 = \omega \varepsilon_0 \mu_0 \]  \hspace{1cm} (24)
\[ \eta_0 = \mu_0 / \varepsilon_0 \]  \hspace{1cm} (25)

If the waveguide is isotropic, namely K_{xx} = K_{yy} = K_{zz} = n^2 and K_{xy} = K_{xz} = K_{yz} = 0, (20) is reduced to the Helmholtz equation for the TE_{0} mode (E_{z} = 0) and (21) is reduced to that for the TM_{0} mode (H_{y} = 0) derived by Yasuura, Shimohara, and Miyamoto [20], where n is the refractive index. In the case of an infinite slab waveguide (\partial/\partial x = 0), two-dimensional waveguide) [14]–[17], the approximate basic equations (20) and (21) are reduced to the exact equations for the two-dimensional guided modes.

III. FINITE-ELEMENT APPROACH

The finite-element formulation is based on the following variational expression [2], [3], [5]–[8], [18] for previous
equations (20) and (21):
\[ \delta I = 0 \]

where
\[ I = \int_{\Omega} \left( K_{xx} \frac{\partial \phi^*}{\partial x} \frac{\partial \phi}{\partial x} + K_{xy} \frac{\partial \phi^*}{\partial y} \frac{\partial \phi}{\partial y} \right) + \left[ k_z^2 - k_0^2 \left( K_{xx} - K_{xy} \frac{b_x}{a_x} - K_{zz} \frac{c_x}{a_x} \right) \right] \phi^* \phi \]
\[ + \frac{K_{zz}}{a} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \frac{K_{yy}}{a} \frac{\partial \psi^*}{\partial y} \frac{\partial \psi}{\partial y} + \left( k_z^2 - k_0^2 \right) \psi^* \psi \]
\[ + j k_z \frac{K_{yz}}{a} \left( \psi^* \frac{\partial \psi}{\partial y} - \frac{\partial \psi^*}{\partial y} \psi \right) \]
\[ + k_0 k_z \frac{b_x}{a_x} \left( \phi^* \frac{\partial \psi}{\partial y} - \frac{\partial \psi^*}{\partial y} \psi \right) \]
\[ - j k_0 \frac{c_x}{a_x} \left( \phi \frac{\partial \psi}{\partial y} - \frac{\partial \phi}{\partial y} \psi \right) \]
\[ dx \, dy. \]

Here, \( \Omega \) is the cross section of the guide and the asterisk denotes complex conjugate.

Dividing the cross section of the guide into a number of 2nd-order triangular elements as shown in Fig. 2, \( \phi \) and \( \psi \) in (23) within each element are defined in terms of \( \phi_k \) and \( \psi_k \) at the nodal points \( k (k = 1, 2, \ldots, 6) \), respectively, as follows:
\[ \phi = \{ N \}^T \{ \phi \}_e \]
\[ \psi = \{ N \}^T \{ \psi \}_e \]
\[ \{ \phi \}_e = [\phi_1 \phi_2 \phi_3 \phi_4 \phi_5 \phi_6]^T \]
\[ \{ \psi \}_e = [\psi_1 \psi_2 \psi_3 \psi_4 \psi_5 \psi_6]^T \]
\[ \{ N \}_e = [N_1 N_2 N_3 N_4 N_5 N_6]^T. \]

Here \( T \), \( \{ \cdot \} \), and \( \{ \cdot \}^T \) denote a transpose, a column vector, and a row vector, respectively, and the shape functions \( N_1 \) to \( N_6 \) are given by
\[ N_1 = L_1 (2L_1 - 1) \]
\[ N_2 = L_2 (2L_2 - 1) \]
\[ N_3 = L_3 (2L_3 - 1) \]
\[ N_4 = 4L_1 L_2 \]
\[ N_5 = 4L_2 L_3 \]
\[ N_6 = 4L_1 L_3 \]

with the area coordinates \( L_1 \), \( L_2 \), and \( L_3 \) [2], [5]. The relation equation between the area coordinates and Cartesian coordinates is given by
\[ \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & x_3 & 1 \\ y_1 & y_2 & y_3 & 1 \end{bmatrix} \begin{bmatrix} L_1 \\ L_2 \\ L_3 \end{bmatrix} \]
(34)

where \( (x_i, y_i) \) are the Cartesian coordinates of the vertex \( i \) \( (i = 1, 2, 3) \) of the triangle.

Both \( \phi \) and \( \psi \) fields exist in the medium (or media) surrounding the optical waveguide, and these fields extend to infinity. One method for modeling the surround is imposing an artificial zero boundary condition for \( \phi \) and \( \psi \) at a large enough distance from the guide. This method has as an advantage its simplicity and is widely used [2]–[8], [12], [13]. Using this zero boundary condition and substituting (28) and (29) into (27), from (26) we obtain the following global matrix equation:
\[ \begin{bmatrix} [A] & [B] \\ [C] & [D] \end{bmatrix} \{ \phi \}_e = \{ 0 \} \]
(35)

where
\[ [A] = \sum_e \int_{\Omega_e} \left( K_{xx} \frac{\partial \{ N \}}{\partial x} \frac{\partial \{ N \}}{\partial x} + \frac{\partial \{ N \}}{\partial y} \frac{\partial \{ N \}}{\partial y} \right) \]
\[ + \frac{K_{yy}}{a} \frac{\partial \{ N \}}{\partial y} \frac{\partial \{ N \}}{\partial y} \]
\[ + \left( k_z^2 - k_0^2 \right) \frac{\partial \{ N \}}{\partial y} \frac{\partial \{ N \}}{\partial y} \]
\[ \cdot \{ N \} \{ N \}^T \] dx \, dy \]
(36a)

\[ [B] = \sum_e \int_{\Omega_e} \left( k_0 k_z \frac{b_x}{a_x} \{ N \} \{ N \}^T \right) \]
\[ - j k_0 \frac{c_x}{a_x} \{ N \} \frac{\partial \{ N \}}{\partial y} \] dx \, dy \]
(36b)

\[ [C] = \sum_e \int_{\Omega_e} \left( k_0 k_z \frac{b_x}{a_x} \{ N \} \{ N \}^T \right) \]
\[ + j k_0 \frac{c_x}{a_x} \frac{\partial \{ N \}}{\partial y} \{ N \} \] dx \, dy \]
(36c)

\[ [D] = \sum_e \int_{\Omega_e} \left( K_{zz} \frac{\partial \{ N \}}{\partial x} \frac{\partial \{ N \}}{\partial x} \right) \]
\[ + K_{yy} \frac{\partial \{ N \}}{\partial y} \frac{\partial \{ N \}}{\partial y} \]
\[ + j k_z \frac{K_{yz}}{a_x} \left( \{ N \} \frac{\partial \{ N \}}{\partial y} - \frac{\partial \{ N \}}{\partial y} \{ N \} \right) \] dx \, dy. \]
(36d)

Here the summation \( \sum_e \) extends over all different elements, the components of \( \{ \phi \} \) and \( \{ \psi \} \) vectors are the values of \( E_x \) and \( \eta_0 H_z \) at nodal points in \( \Omega \), respectively, and \( \{ 0 \} \) is a null vector.

For an anisotropic waveguide with a diagonal permittivity tensor, namely \( K_{xx} = K_{yz} = K_{yy} = 0 \), (35) is reduced to the equations derived by Koshiba, Hayata, and Suzuki [12]. In this case, \( [B] = [C] = [0] \) (where \( [0] \) is a zero matrix) and
equations $[A] = 0$ and $[B] = 0$ determine the dispersion characteristics for the $E_x^p$ and $E_y^p$ modes [10] in the waveguides with a diagonal permittivity tensor, respectively. The main field components of the $E_x^p$ modes are $E_x$ and $H_y$, while those of the $E_y^p$ modes are $H_x$ and $E_y$ [10]. The subscripts $p$ and $q$ are used to designate the number of maxima of the dominant field in the $x$- and $y$-directions, respectively. In the case of a two-dimensional waveguide ($\partial/\partial x = 0$), (35) gives the exact expression for two-dimensional guided modes [18], [19].

In order that a nontrivial solution of (35) may exist

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = 0 \quad (37)$$

must hold. This equation is the eigenvalue (dispersion) equation which determines the dispersion characteristics for the guided modes in anisotropic waveguides having a permittivity tensor with nonzero off-diagonal elements. In the present analysis, the Cholesky method, the Householder's method, the method of bisections, and the QR method are suitably used for solving (37).

IV. COMPUTED RESULTS

Equation (12) and neglect of $E_y$ and $H_y$ in (20) and (21) may not be valid for the neighborhood of cutoff frequency and for the higher order modes. Therefore, it is necessary to study the accuracy of the method.

First we consider isotropic dielectric waveguides which are analyzed by many researchers using a variety of methods [1]-[13], [20]. Fig. 3 shows the dispersion characteristics for the fundamental $E_{11}^p$ mode in an embossed waveguide and in a channel waveguide, where the index variation in the lateral direction of the channel waveguide is smaller than that of the embossed waveguide and the finite-element model uses 84 elements and 195 nodal points in one-half of the cross section. For the embossed waveguide, our results (solid lines) deviate from the results (dots) of the vectorial finite-element method [5] in the neighborhood of cutoff frequency when the width $W/t$ is narrow ($W/t = 1$ and 2). On the other hand, for the channel waveguide with $W/t = 2$, agreement between our results (dashed line) and the results (circles) of the vectorial finite-element method is good over a wide range of frequencies. In [12], the approximate scalar finite-element method is used for the analysis of an anisotropic channel waveguide with a diagonal permittivity tensor and a 1-percent variation of the ordinary and extraordinary refractive indices of LiNbO$_3$, and the results obtained agree very well with the results of the vectorial finite-element method [3].

Fig. 4(a) shows the dispersion characteristics for the $E_x^p$ and $E_y^p$ modes in a rib waveguide, where the finite-element model employs 180 elements and 399 nodal points in one-half of the cross section. The $E_{11}^p$ (or $E_{21}^p$) and $E_{12}^p$ (or $E_{22}^p$) modes are the lowest modes of the symmetric ($p$ is odd) and antisymmetric ($p$ is even) $E_x^p$ (or $E_y^p$) modes, respectively. Our results for these modes agree well with the results of the mode-matching method [20]. However, our results for the higher order $E_x^p$ and $E_y^p$ modes are not in good agreement with the results of the mode-matching method, especially near the cutoff frequencies. Fig. 4(b) shows the dispersion characteristics for the fundamental $E_{11}^p$ mode in the rib waveguide when the width $W/t$ is altered. When the width $W/t$ becomes narrow, our results deviate from the results (dots) of the mode-matching method. But our results are closer to the results of the mode-matching method than those (circles) of Marcatili's approximate analytical approach [10]. From Figs. 3 and 4, we may conclude that the approximate scalar finite-element results are more accurate for the lower order modes in the waveguide of a small index variation in the lateral direction.
As for the second example, we consider an anisotropic dielectric rectangular waveguide composed of a uniaxial medium. A typical division of this waveguide into 2nd-order triangular elements is shown in Fig. 5, where the number of elements and of nodal points is 80 and 169, respectively. Figs. 6–8 show the dispersion characteristics for the guided modes in the anisotropic dielectric rectangular waveguides surrounded by an isotropic medium of refractive index \( \sqrt{2.05} \), where the ordinary and extraordinary refractive indices of a rectangular core are \( \sqrt{2.31} \) and \( \sqrt{2.19} \), respectively. The optic axis \( c \) in Figs. 6, 7, and 8 lies in the \( xy \)-plane at an angle \( \theta = 45^\circ \) from the \( x \)-axis \( (K_{xy} \neq 0, K_{xz} = K_{yz} = 0) \), in the \( xz \)-plane at an angle \( \theta = 45^\circ \) from the \( z \)-axis \( (K_{xz} \neq 0, K_{xy} = K_{yz} = 0) \), and in the \( yz \)-plane at an angle \( \theta = 45^\circ \) from the \( z \)-axis \( (K_{yz} \neq 0, K_{xy} = K_{xz} = 0) \), respectively. Modes are designated as \( E_{pq}^{\pm} \) (\( E_{pq}^{\pm} \)-like mode).
if at a frequency near cutoff the electric field \( E_x \) is dominant and as \( E_{pq} \) (\( E_{pq} \)-like mode) if at a frequency near cutoff the magnetic field \( H_x \) is dominant. As we can see from (35) and (36), in general, there is coupling between the field components \( E_x \) and \( H_x \) via the off-diagonal element \( K_{ij} \). In the case of \( K_{yz} \neq 0 \) and \( K_{xy} = K_{xz} = 0 \) in Fig. 8, the matrices \([B]\) and \([C]\) in (35) vanish, and the \( E_{pq} \)-modes group and the \( E^{p}_{jq} \)-modes group are separable in the present approach. For the waveguide in Fig. 6, the region \( ABCD \) in Fig. 5 should be divided into elements because of the lack of symmetry of the field. The waveguide in Fig. 7 or 8 has a plane of symmetry, \( y = t/2 \) or \( x = 0 \), respectively. Therefore, for the waveguide in Fig. 7 or 8 the region \( ABGH \) or \( AEFD \) in Fig. 5 is divided into elements, respectively.

Ohtaka [11] has analyzed the anisotropic dielectric rectangular waveguide with \( W = 2t \) whose optic axis lies in the \( xy \)-plane using the variational method. Comparison of our results for the waveguide in Fig. 6(a) with the results of the vectorial wave analysis using the variational method shows good agreement. This fact demonstrates the reliability of the present method. With reference to Figs. 6-8, effects of the direction of the optic axis and the guide-width on the dispersion characteristics of the guided modes can be observed. In the waveguide whose optic axis lies in the \( xy \)-plane, the fundamental mode is the \( E_{x}^s \)-mode and in the waveguide whose optic axis lies in the \( xz \)-plane the fundamental mode is \( E_{x}^t \)-mode. When the guide-width is made narrower, the cutoff frequency of each mode becomes higher and the frequency range of single-mode operation in each class of modes (the \( E^{p}_{pq} \)-like modes and the \( E^{p}_{pq} \)-like modes) becomes wider.

The nonphysical spurious solutions do not appear in Figs. 3, 4, and 6-8 because of the positive definite nature of (27).

V. Conclusions

An approximate scalar finite-element method was developed for the analysis of three-dimensional anisotropic optical waveguides having a permittivity tensor with nonzero off-diagonal elements. In this approach, the nonphysical spurious solutions which are included in the solutions of the vectorial finite-element method in an axial components formulation do not appear.

The present approach may be applicable to the analysis of three-dimensional anisotropic diffused optical waveguides.

In the present approach, the artificial zero boundary condition is used at a large enough distance from the guide (bounded structure), so the entire mode spectrum is a discrete set of modes. The problem of how to deal with an open guided-wave structure (unbounded structure), including the continuous spectrum hereafter still remains.

REFERENCES


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