An Effective Method for Calculating the Waveguide and Leaky Modes of a Planar Multilayer Structure

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Abstract. The paper proposes a new method for calculating the waveguide and leaky modes when passing EM waves through a planar multilayer anisotropic structure having dielectric and magnetic permeability described by diagonal tensors. On the basis of the Transformation Matrix (TMM) Method applied at three neighboring points, a difference equation is constructed, summarized simultaneously for TE and TM modes. Its coefficient matrix contains trigonometric functions and has a tridiagonal structure. To find the propagation constants, we approximate the coefficients of the equation by using a finite number of terms of Maclaurin series and we reach the solution of the eigenvalue problem and vectors of the form $\mathbf{A}u = \lambda^n \mathbf{B}u + \lambda^{n-1}\mathbf{C}u + \cdots + \lambda \mathbf{Z}u$, reduced by suitable substitutions to a generalized linear problem $\tilde{\mathbf{A}}u = \lambda \tilde{\mathbf{B}}u$. The solution is obtained by using the dynamic shifted inverse power method with Rayleigh quotient. The exact number of roots of interest bounded by a closed rectangular contour C in the complex plane is determined by the value of $\frac{1}{2\pi i}\oint_C \frac{f'(z)}{f(z)}dz = N - P$, where N is the number of roots, P is the number of poles, $f'(z)$ is the first derivative of the function $f(z)$ and $f(z)=0$ represented the dispersion transcendental equation obtained by the TMM method. When comparing the results by the two methods, we replaced the solution of the dispersion equation by finding the zeros of an approximation polynomial having the same roots in the area bounded by contour C.

Keywords: waveguide, numerical methods, multilayer planar waveguide, mode solver.

1. INTRODUCTION

Planar multilayer waveguide structures are often incorporated into various instruments of integrated optics. The use of a fast and efficient method for calculating the modes of such a structure is of particular importance in developing them. The TMM transformation matrix method [.., ..] is convenient for use in structures with a small number of layers. The propagation constants are the roots of the transcendental dispersion equation. Solving this equation poses great mathematical difficulties due to the occurrence of rounding errors and the appearance of additional false roots. The finite difference methods FD, FDTD, FDED are easy to work with. They lead to the solution of linear algebraic systems of equations $\mathbf{A}u = \lambda u$ where matrix A has a band structure. They give good accuracy when calculating maximum modulus propagation constants, but not particularly good at smaller. A huge number of points need to be taken for layers with very different refractive indices. There are also unnecessary roots.

This paper proposes a method that combines the benefits of both TMM and FD approaches. The problem of redundant roots is solved by proposing a formula for the number of roots of the dispersion equation in the closed area of interest of the complex plane. Rounding errors are significantly reduced by replacing the solution of the dispersion transcendental equation by searching for the roots of an approximation polynomial having the same roots in the domain.

2. THEORETICAL BASIS

2. 1. Physical Model

Let the planar anisotropic waveguide structure characterized by diagonal dielectric and magnetic permeability tensors [ε] and [μ] are oriented, as shown in Fig. 1. With j we denote the number of layers, with d_j their thickness, a polarized EM wave propagates through their media in the direction of the 0z axis, with a time-constant configuration with frequency ω and a propagation constant β.

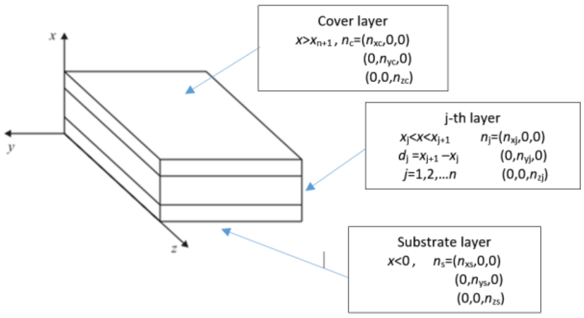

Fig. 1 Multilayer planar waveguide structure.

The description for each layer is done by the system:

$$\begin{pmatrix} 0 & i\beta & \partial/\partial y \\ -i\beta & 0 & -\partial/\partial x \\ -\partial/\partial y & \partial/\partial x & 0 \end{pmatrix} \begin{pmatrix} E_{xj} \\ E_{yj} \\ E_{zj} \end{pmatrix} = -i\omega\mu_0 \begin{pmatrix} \mu_{xj} & 0 & 0 \\ 0 & \mu_{yj} & 0 \\ 0 & 0 & \mu_{zj} \end{pmatrix} \begin{pmatrix} H_{xj} \\ H_{yj} \\ H_{zj} \end{pmatrix} \quad (1a)$$

$$\begin{pmatrix} 0 & i\beta & \partial/\partial y \\ -i\beta & 0 & -\partial/\partial x \\ -\partial/\partial y & \partial/\partial x & 0 \end{pmatrix} \begin{pmatrix} H_{xj} \\ H_{yj} \\ H_{zj} \end{pmatrix} = i\omega\varepsilon_0 \begin{pmatrix} \varepsilon_{xj} & 0 & 0 \\ 0 & \varepsilon_{yj} & 0 \\ 0 & 0 & \varepsilon_{zj} \end{pmatrix} \begin{pmatrix} E_{xj} \\ E_{yj} \\ E_{zj} \end{pmatrix} \quad (1b)$$

For TE modes $\vec{E} = (0, E_{yj}(x,z), 0)$ considering magnetic permeability [μ] we have

$$\mu_{xj} \frac{\partial}{\partial x}\left(\frac{1}{\mu_{zj}} \frac{\partial}{\partial x} E_{yj} \right) + \left(\omega^2 \varepsilon_0 \varepsilon_{yj} \mu_0 \mu_{xj} \right) E_{yj} = \beta^2 E_{yj} \quad (2)$$

$$H_{xj} = -\frac{\beta}{\omega\mu_0\mu_{xj}} E_{yj}, \quad H_{zj} = \frac{i}{\omega\mu_0\mu_{zj}} \frac{\partial}{\partial x} E_{yj} \quad (3)$$

For TE modes $\vec{H} = (0, H_{yj}(x,z), 0)$ considering magnetic permeability [μ] we have

$$\varepsilon_{xj} \frac{\partial}{\partial x}\left(\frac{1}{\varepsilon_{zj}} \frac{\partial H_{yj}}{\partial x} \right) + \left(\omega^2 \varepsilon_0 \varepsilon_{xj} \mu_0 \mu_{yj} \right) H_{yj} = \beta^2 H_{yj} \quad (4)$$

$$E_{xj} = \frac{\beta}{\omega\varepsilon_0\varepsilon_{xj}} H_{yj}, \quad E_{zj} = -\frac{i}{\omega\varepsilon_0\varepsilon_{zj}} \frac{\partial}{\partial x} H_{yj} \quad (5)$$

The total electric and magnetic field for all layers is of the form:

$$E_y(x,z) = \sum_{j=1}^{n} E_{yj}(x,z) = u(x) e^{-i\beta z}, \quad (6)$$

$$H_y(x,z) = \sum_{j=1}^{n} H_{yj}(x,z) = u(x) e^{-i\beta z}. \quad (7)$$

In this way, equations (2) and (4) are converted into ordinary second-order differential equations with unknown function $u(x)$.

Let by function $n(x) = \{n_x(x), n_y(x), n_z(x)\}$ we denote the refractive indices covering all layers.

2. 2. A Combined Method for TE and TM Modes

There is a relation between the representation of the solutions $u(x)$ by TMM method at three adjacent points x_{j-1}, x_j, x_{j+1} (or three consecutive layers) and therefore for all n layers coincides with the solution of the following nonlinear transcendental difference equation.

$$\left[\frac{1}{\eta_j} \frac{\Delta_j d_j}{\sin(\Delta_j d_j)} \frac{u_{j+1} - u_j}{d_j} - \frac{1}{\eta_{j-1}} \frac{\Delta_{j-1} d_{j-1}}{\sin(\Delta_{j-1} d_{j-1})} \frac{u_j - u_{j-1}}{d_{j-1}} \right] \frac{2}{d_j + d_{j+2}} + \left[\frac{1}{\eta_j} \Delta_j^2 \frac{tg(\Delta_j d_j/2)}{\Delta_j d_j/2} + \frac{1}{\eta_{j-1}} \Delta_{j-1}^2 \frac{tg(\Delta_{j-1} d_{j-1}/2)}{\Delta_{j-1} d_{j-1}/2} \right] u_j = 0 \quad (6)$$

where $u_j = u(x_j)$, $d_j = x_{j+1} - x_j$, $\Delta_j^2 = k_0^2 n^2(x_j) - \beta^2$ $\eta_j = 1$ for TE modes and $\eta_j = 1/n^2(x_j)$ for TM modes.

In order to avoid solving the nonlinear transcendental problem, we propose the decomposition of the coefficients containing trigonometric functions in the series of Maclaurin:

$$\frac{d_j \Delta_j}{\sin(d_j \Delta_j)} = 1 + \frac{1}{6}\left(d_j \Delta_j\right)^2 + \frac{7}{36}\left(d_j \Delta_j\right)^4 + \cdots \quad (7)$$

$$\frac{tg(d_j \Delta_j/2)}{(d_j \Delta_j/2)} = 1 + \frac{1}{12}\left(d_j \Delta_j\right)^2 + \frac{1}{144}\left(d_j \Delta_j\right)^4 + \cdots \quad (8)$$

Taking into account only the first term of the series, the system goes into the standard eigenvalue and eigenvector problem $\mathbf{A}u = \lambda u$ obtained by the FD finite difference method, where the divisions are fixed and exactly match the thicknesses of the layers. This method is highly inaccurate, especially with large differences in the thickness of the individual layers of the structure.

Using first and second terms, we obtain an algebraic system of the form $\mathbf{A}u = \lambda^2\mathbf{B}u + \lambda\mathbf{C}u$ and by the substitution $w = \lambda u$ it is reduced to a generalized linear problem $\tilde{\mathbf{A}}u = \lambda\tilde{\mathbf{B}}u$ looking the way

$$\begin{pmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{I} \end{pmatrix}\begin{pmatrix} u \\ w \end{pmatrix} = \lambda\begin{pmatrix} \mathbf{C} & \mathbf{B} \\ \mathbf{I} & 0 \end{pmatrix}\begin{pmatrix} u \\ w \end{pmatrix} \tag{9}$$

The approximation error is $O\left(\left(d_j\Delta_j\right)^4\right)$.

We continued this idea for problem $\mathbf{A}u = \lambda^n\mathbf{B}u + \lambda^{n-1}\mathbf{C}u + \cdots + \lambda\mathbf{Z}u$ reduced to a standard linear problem $\tilde{\mathbf{A}}u = \lambda\tilde{\mathbf{B}}u$ that way

$$\begin{pmatrix} \mathbf{A} & 0 & \cdots & 0 \\ 0 & \mathbf{I} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & \mathbf{I} \end{pmatrix}\begin{pmatrix} u \\ v \\ \cdots \\ w \end{pmatrix} = \lambda\begin{pmatrix} \mathbf{Z} & \cdots & \mathbf{C} & \mathbf{B} \\ \mathbf{I} & 0 & \cdots & 0 \\ 0 & \mathbf{I} & \cdots & 0 \\ 0 & \cdots & \cdots\mathbf{I} & 0 \end{pmatrix}\begin{pmatrix} u \\ v \\ \cdots \\ w \end{pmatrix} \tag{10}$$

where $\begin{pmatrix} u \\ v \\ \cdots \\ w \end{pmatrix} = \begin{pmatrix} u \\ \lambda u \\ \cdots \\ \lambda^{n-1}u \end{pmatrix}$, $\mathbf{I}$ is the identity matrix.

The approximation error we make after counting the first "n" terms is $O\left(\left(d_j\Delta_j\right)^{n+2}\right)$.

2. 3. Determining the Number of Roots of the Dispersion Equation

If the function $f(z)$ is analytic and does not go to zero over a closed integral contour, then argument principle has the form:

$$S_0 = \frac{1}{2\pi i}\oint_C \frac{f'(z)}{f(z)}dz = N - P \tag{11}$$

where N is the numbers of zeros and P is number of poles inside the region enclosed by the contour C. Once poles have been identified, which are $\beta = n_c$ and $\beta = n_s$ from dispersion equation obtained by TMM method, rectangular integral contour C is selected for the guided modes and enclose area between the minimum and the maximum real parts of all the refractive indices. It do not enclose any of the poles. For leaky modes integral contour C enclose area between refractive indices of cover layer and substrate (if $n_s > n_c$) or enclose area between 0 and n_s (if $n_s = n_c$) and do not enclose any of them. If there are no poles in region, then S_0 is the number of zeros.

2. 4. Constructing a Polynomial Along the Roots of the Dispersion Equation

According to formula (11) for $P = 0$ we form the sums:

$$S_m = \frac{1}{2\pi i}\oint_C z^m \frac{f'(z)}{f(z)}dz = \sum_{i=0}^{S_0} z_i^m \tag{12}$$

for $m = 1, 2, \cdots, S_0$, where z_i, $i = 1, 2, \cdots, S_0$ are the roots of $f(z)$ inside *C*. It leads to a system of equations that can be used to evaluate the coefficients of approximation polynomial $p(z)$ of degree S_0, which has the some roots $z_1, \cdots, z_{S_0}$.

$$p(z) = \prod_{i=1}^{S_0}\left(z - z_i\right) = \sum_{k=0}^{S_0} C_k z^k \tag{13}$$

where $C_{S_0} = 1$ and other coefficients are given via recursive formula:

$$C_k = \frac{1}{k - S_0}\sum_{j=1}^{S_0-k} S_j C_{k+j}, \; k = S_0 - 1, \cdots, 0 \tag{14}$$

The initial difficult problem of finding of zeros of any dispersion equation is transformed to the problem of finding the zeros of polynomial, for witch a many effective numerical methods exist.

3. NUMERICAL RESULTS

The proposed method was applied to the dielectric four layer planar waveguide structure. Substrate: $n_s = 1.5$, Cover: $n_c = 1.0$ layers: $n_1 = 1.66$, $n_2 = 1.60$, $n_3 = 1.53 - i1.53.10^{-4}$, Thickness: $d_1 = d_2 = d_3 = d_4 = 0.5$ μm, $\lambda = 0.6328$ μm. Results are in the excellent agreement with those reported in reference […] as shown at Table 1. The field distribution of TE modes are shown in Fig. 2.

TABLE 1. Guided TE mode effective indices in a 4-layer planar waveguide structure.

	TMM method		Proposed method		Rzhanov at. All, 2010	
Mode	$\mathrm{Re}\frac{\beta}{k_0}$	$\mathrm{Im}\frac{\beta}{k_0}$	$\mathrm{Re}\frac{\beta}{k_0}$	$\mathrm{Im}\frac{\beta}{k_0}$	$\mathrm{Re}\frac{\beta}{k_0}$	$\mathrm{Im}\frac{\beta}{k_0}$
TE_0	1.62261	$6.73 .10^{-7}$	1.62272	$6.8.10^{-7}$	1.6227	$6.73 .10^{-7}$
TE_1	1.60531	$1.66 .10^{-4}$	1.60499	$1.78 .10^{-4}$	1.6053	$1.66 .10^{-4}$
TE_2	1.55708	$2.11 .10^{-4}$	1.54332	$3.09 .10^{-4}$	1.5571	$2.11 .10^{-4}$
TE_3	1.50349	$5.51 .10^{-5}$	1.51443	$4.351 .10^{-5}$	1.5036	$5.50 .10\text{-}^{5}$

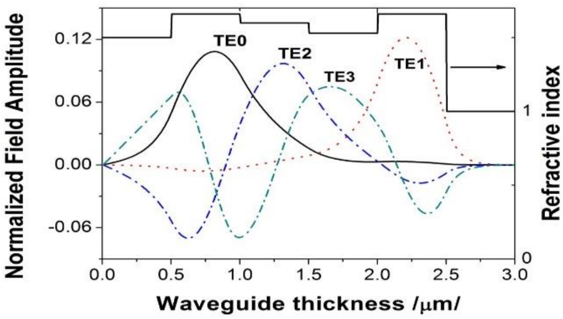

Fig. 2 Field distribution for TE guided modes of 4-layer planar waveguide structure.

The calculations according to the our method are made using two Maclaurin series terms. With the method we propose, a better approximation is observed for the larger eigenvalues. An almost exact coincidence of the results is observed when applying the TMM method with solving the transcendental equation and the TMM method with finding the zeros of the proposed approximation polynomial.

The proposed method was applied to Metal-Clad Waveguide planar structure whose data is taken from […]. The substrate layer $LiNbO_3$ has the largest real part of the refractive index $n_s = 2.2026$ and the cover layer has the smallest real part $n_c = 1.0$. Wavelength is $\lambda_0 = 0.6833\mu m$, layer-1: Ag $n_x = 0.067 + 4.05i$, $n_z = 0.067 + 4.05i$, layer thickness $d_1 = 0.2\lambda_0$; layer-2: ZnO $n_x = 2.007$, $n_2 = 1.990$, thickness $d_2 = 0.54\lambda_0$; layer-3: $PELiNbO_3$ $n_x = 2.3266$, $n_z = 2.2465$, thickness $d_3 = 1.33\lambda_0$.

The integration contour in the complex plane must exclude point 2.2026 because it is a pole. Therefore, the propagation constants will have a larger real part for waveguide modes and real parts between 1 and 2.2026 for leaky modes. We will only illustrate the waveguide modes here.

In the calculations, we used the difference equation of the proposed method, transforming it into a generalized linear problem according to formula (10) using the expansions of the trigonometric functions in the series of Maclaurin limited to 3 terms. The total number of divisions for all layers is 1024. The results for the most significant modes are shown in Table 2. The normalized field distribution are shown in Fig. 3.

The results of proposed method shows good accuracy for the real parts and not particularly good for the imaginary ones. The results of TMM method with approximation polynomial exactly matches the ones mentioned in (Offersgaard, 1995.

TABLE 2. Normalized propagation constants of a plane waveguide structure air / Ag / ZnO / PELiNbO3 / LiNbO3.

	TMM method		Proposed method		Offersgaard J. F., 1995	
Mode	$\mathrm{Re}\frac{\beta}{k_0}$	$\mathrm{Im}\frac{\beta}{k_0}$	$\mathrm{Re}\frac{\beta}{k_0}$	$\mathrm{Im}\frac{\beta}{k_0}$	$\mathrm{Re}\frac{\beta}{k_0}$	$\mathrm{Im}\frac{\beta}{k_0}$
TM_0	2.30557	0.0119	2.3050	0.0123	2.30557	0.01186
TM_1	2.30556	0.0003	2.3050	0.0020	2.30556	0.00026
TM_2	2.24998	0.0001	2.2420	0.0002	2.24500	0.00006

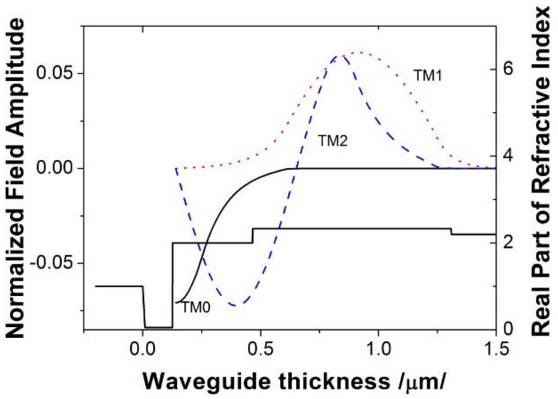

Fig. 3 Field distribution for TM modes of air/Ag/ZnO/PELiNbO3/LiNbO3 structure.

It is interesting in this example that the real parts of the propagation constants of TM_0 and TM_1 are almost identical, but the imaginary ones are in two orders of magnitude. This could mean that the losses for TM_1 are much smaller than the basic one. Their eigenvalue is approximately equal to the surface plasmon mode (wavelength) occurring at the ZnO-Ag boundary.

Both methods produce acceptable results, the direct TMM method with approximation polynomial is more accurate, while the method proposed by us is faster and requires less machine time.

4. CONCLUSION

A method was proposed that transforms the Transform Matrix Method (TMM) into a Finite Difference Method (FD). Coefficients of difference equation containing trigonometric functions are decomposed in Maclaurin series, using one, two or more terms and then proceeds to the generalized linear eigenvalue problem $Au = \lambda Bu$. The matrices A and B have are banded form.

An algorithm was proposed for finding the roots of transcendental equations and specifying their number in a closed rectangular contour in the complex plane by replacing them with an approximation polynomial having the same roots, while at the same time we were able to find dependencies for the real parts of the refractive indices for the waveguide and leaky modes.

The proposed methods have been verified by calculating the modes of a waveguide structure with dielectric layers and a waveguide structure comprising metal, dielectric and semiconductor layers.

The results show higher accuracy of TMM with approximation polynomial, but better performance of the proposed difference method.

Both methods are suitable for engineering calculations in the design of multilayer waveguide structures.

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