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Improved Finite-Difference Beam-Propagation Method Based on the Generalized Douglas Scheme and Its Application to Semivectorial Analysis

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Abstract—The generalized Douglas scheme for variable coefficients is applied to the propagating beam analysis. Once the alternating direction implicit method is used, the truncation error is reduced in the transverse directions compared with the conventional Crank–Nicholson scheme, maintaining a tridiagonal system of linear equations. Substantial improvement in the accuracy is achieved even in the TM mode propagation. As an example of the semivectorial analysis, the propagating field and the attenuation constant of a bent embedded waveguide with a trench section are calculated and discussed.

I. INTRODUCTION

THE beam-propagation method (BPM) is widely used to design various optical circuits. In addition to the BPM based on the fast Fourier transform [1], the finite difference techniques are also applied to the propagating beam analysis [2]–[6]. It is well known that the implicit method such as the Crank–Nicholson (CN) scheme allows the use of a larger propagation step length Δz than the explicit method. The CN scheme has an advantage of unconditional stability, although the truncation error is $O(\Delta x)^2$ in the transverse direction.

To improve the accuracy, Yevick *et al.* [7] first introduced the Douglas scheme [8] into the propagating beam analysis. They applied the Douglas scheme to the Fresnel equation with the phase term being split. The truncation error is reduced to $O(\Delta x)^4$. It should be noted, however, that splitting the phase term results in the fact that the step length Δz must be small. We can expect a larger step length when the phase term is not split [9].

Recently, we have formulated the modified finite-difference beam-propagation method (FD–BPM) based on the generalized Douglas (GD) scheme for variable coefficients [10], with the phase term being not split. The accuracy of our formulation is better than that of the previous one derived by Sun and Yip [11], maintaining the advantage that the result is not a sensitive function of Δz . The truncation error of $O(\Delta x)^4$ is ensured in the transverse direction.

The purpose of this paper is to discuss the application of the GD scheme to the propagating beam analysis in more detail. The GD scheme is applied to a semivectorial FD–BPM using the alternating direction implicit method (ADIM) [12]–[15]. Although the GD scheme holds approximately true in the

semivectorial FD–BPM, it still gives substantial improvement in the accuracy, as compared with the conventional CN scheme.

After demonstrating reduction of the mode-mismatch loss in a step-index waveguide, we present numerical results of a three-dimensional embedded optical waveguide. Properties of quasi-TE and quasi-TM polarized modes are investigated by solving a semivectorial equation. The field distributions of a bent embedded waveguide are evaluated and the effects of a trench section [16]–[20] on the attenuation constant are discussed.

II. SCALAR FORMULATION

We first summarize the GD scheme in a two-dimensional problem. The Fresnel equation for the propagating beam problem is expressed as

$$\sigma \frac{\partial E}{\partial z} = \frac{\partial^2 E}{\partial x^2} + \nu E \quad (1)$$

where $\sigma = 2jk n_0$ and $\nu = k^2[n^2(x, z) - n_0^2]$, in which k is the free space wavenumber, $n(x, z)$ is the index profile of the waveguide, and n_0 is the reference index to be appropriately chosen.

The philosophy behind the Douglas scheme is to eliminate the truncation error term of the order Δ^2 where Δ is the transverse sampling width. When the truncation error is included, by Taylor's series expansion the second derivative of function E with respect to x is expressed as

$$\frac{\partial^2 E}{\partial x^2} = \frac{\delta^2 E}{\Delta x^2} - \frac{1}{12} \frac{\partial^4 E}{\partial x^4} \Delta x^2 + O(\Delta x)^4. \quad (2)$$

In the conventional CN scheme, only the first term in the right-hand side of (1) is evaluated, so that the truncation error is $O(\Delta x)^2$.

To reduce the truncation error, we substitute (1) into (2), replacing $\partial^4 E / \partial x^4$ with $\delta^2(\sigma \partial E / \partial z - \nu E) / \Delta x^2 + O(\Delta x)^2$. Then, the following difference equation can be derived:

$$\begin{aligned} \frac{(\delta^2 E)}{\Delta x^2} &= \frac{1}{12} \left(\sigma \frac{\partial E}{\partial z} \right)_{i+1} + \frac{5}{6} \left(\sigma \frac{\partial E}{\partial z} \right)_i \\ &+ \frac{1}{12} \left(\sigma \frac{\partial E}{\partial z} \right)_{i-1} - \frac{1}{12} (\nu E)_{i+1} - \frac{5}{6} (\nu E)_i \\ &- \frac{1}{12} (\nu E)_{i-1} + O(\Delta x)^4. \end{aligned} \quad (3)$$

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We now introduce the z differencing and get

$$\begin{aligned} & \frac{\sigma}{12} \frac{E_{i+1}^{l+1} - E_{i+1}^l}{\Delta z} + \frac{5\sigma}{6} \frac{E_i^{l+1} - E_i^l}{\Delta z} + \frac{\sigma}{12} \frac{E_{i-1}^{l+1} - E_{i-1}^l}{\Delta z} \\ &= \frac{(\delta^2 E)_i^{l+1} + (\delta^2 E)_i^l}{2(\Delta x)^2} + \frac{1}{24} [(\nu E)_{i+1}^{l+1} + (\nu E)_{i+1}^l] \\ & \quad + \frac{5}{12} [(\nu E)_i^{l+1} + (\nu E)_i^l] + \frac{1}{24} [(\nu E)_{i-1}^{l+1} + (\nu E)_{i-1}^l] \\ & \quad + O(\Delta z)^2 + O(\Delta x)^4. \end{aligned} \quad (4)$$

As a result, we obtain the following high accuracy six-point scheme:

$$\begin{aligned} & \zeta_{i-1}^- E_{i-1}^{l+1} + \zeta_i^- E_i^{l+1} + \zeta_{i+1}^- E_{i+1}^{l+1} \\ &= \zeta_{i-1}^+ E_{i-1}^l + \zeta_i^+ E_i^l + \zeta_{i+1}^+ E_{i+1}^l \end{aligned} \quad (5)$$

where

$$\begin{aligned} \zeta_i^\pm &= \frac{jk n_0}{6} \pm \frac{\Delta z}{2\Delta x^2} \pm \frac{\nu_i \Delta z}{24} \\ \zeta_i^\pm &= \frac{5jk n_0}{3} \mp \frac{\Delta z}{\Delta x^2} \pm \frac{5\nu_i \Delta z}{12}. \end{aligned}$$

It should be noted that the term ν is a variable coefficient. Inclusion of the $\nu_{i\pm 1}$ terms is significant for the reduction in the truncation error, as have been discussed previously [10]. Equation (4) can be regarded as the Douglas scheme generalized for variable coefficients. The six-point scheme allows us to use an efficient computing algorithm such as the Thomas algorithm, so that the computational speed is almost identical to that in the conventional FD-BPM [3] based on the CN scheme.

The scalar Fresnel equation in three-dimensional (3-D) coordinates are as follows:

$$\sigma \frac{\partial E}{\partial z} = \frac{\partial^2 E}{\partial x^2} + \frac{\partial^2 E}{\partial y^2} + \nu E \quad (6)$$

where it is difficult to directly derive a high-accuracy scheme. As described in [21], the difficulty arises from the fact that $(1/12)\Delta^4(\partial^4 E/\partial x^4 + \partial^4 E/\partial y^4)$ cannot be expressed in terms of the Laplacian of E in a square net of points in the x - y plane. To obtain a high-accuracy scheme, we have to adopt a hexagonal net of points. This results in a 14-point scheme.

It should be noted, however, that once the Peaceman-Rachford ADIM [8], [12] is used, a high accuracy scheme can be obtained. The difference equation corresponding to (6) becomes

$$\begin{aligned} \sigma \frac{E^{l+1} - E^l}{\Delta z} &= \frac{\delta_x^2 E^{l+1} + \delta_x^2 E^l}{2\Delta x^2} + \frac{\delta_y^2 E^{l+1} + \delta_y^2 E^l}{2\Delta y^2} \\ & \quad + \nu \frac{E^{l+1} + E^l}{2}. \end{aligned} \quad (7)$$

We divide the propagation step into two steps of size $\Delta z/2$

$$\sigma \frac{E^{l+1/2} - E^l}{\Delta z/2} = \frac{\delta_x^2 E^{l+1/2}}{\Delta x^2} + \frac{\delta_y^2 E^l}{\Delta y^2} + \nu \frac{E^{l+1/2} + E^l}{2} \quad (8)$$

$$\begin{aligned} \sigma \frac{E^{l+1} - E^{l+1/2}}{\Delta z/2} &= \frac{\delta_x^2 E^{l+1/2}}{\Delta x^2} + \frac{\delta_y^2 E^{l+1}}{\Delta y^2} \\ & \quad + \nu \frac{E^{l+1} + E^{l+1/2}}{2}. \end{aligned} \quad (9)$$

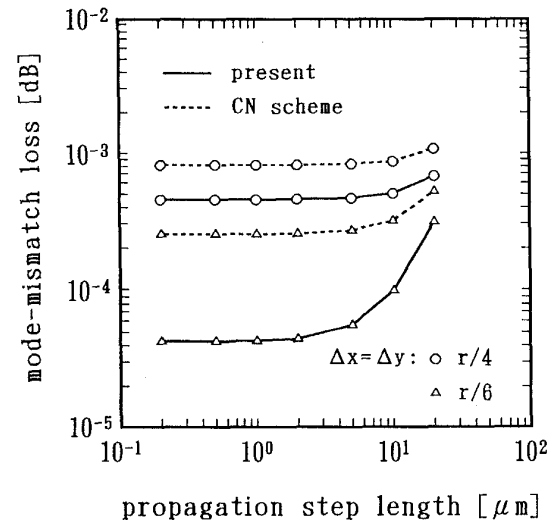


Fig. 1. Mode-mismatch loss for a step-index fiber as a function of propagation step length.

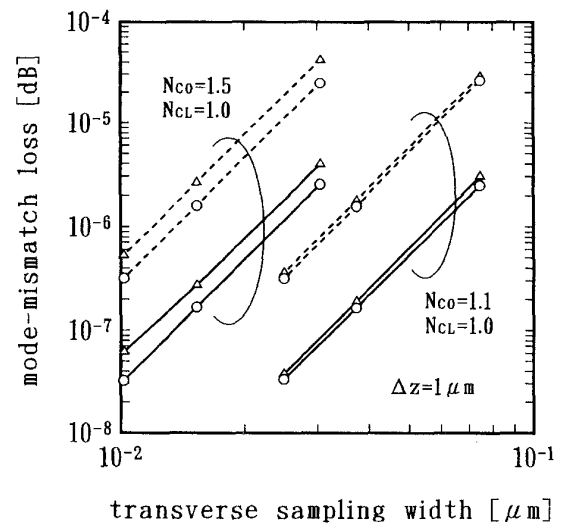


Fig. 2. Mode-mismatch loss for a step-index slab waveguide as a function of transverse sampling width: — present, CN scheme, ○ TE₀ mode, △ TM₀ mode.

Since the treatment regarding the two half-steps is the same, we only discuss the first half-step in the following.

Equation (8) can be separated into

$$\left(\sigma \frac{\partial E}{\partial z} \right)^l = 2 \left(\frac{\partial^2 E}{\partial y^2} \right)^l + \nu E^l, \quad (10)$$

$$\left(\sigma \frac{\partial E}{\partial z} \right)^{l+1/2} = 2 \left(\frac{\partial^2 E}{\partial x^2} \right)^{l+1/2} + \nu E^{l+1/2}. \quad (11)$$

This is confirmed by the fact that the integration of $\sigma(\partial E/\partial z)$ in the interval $[z, \Delta z/2]$ using (10) and (11) results in (8). Since the forms of (10) and (11) are almost the same as (1), we can use the GD scheme even in a 3-D problem. The efficient

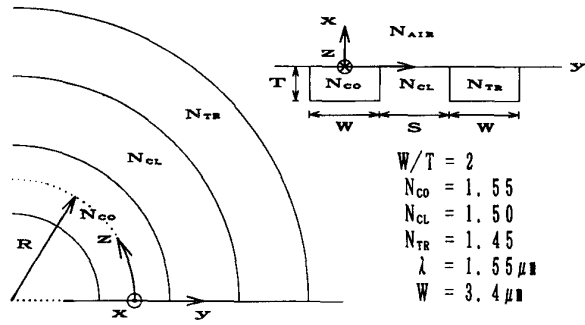


Fig. 3. Configuration of a bent embedded optical waveguide.

computing algorithm can again be used as in the case of a two-dimensional problem. As a result, the following difference equations split into two steps are derived:

$$\begin{aligned} & \zeta_{x\,i-1,j}^- E_{i-1,j}^{l+1/2} + \xi_{x\,i,j}^- E_{i,j}^{l+1/2} + \zeta_{x\,i+1,j}^- E_{i+1,j}^{l+1/2} \\ & = \zeta_{y\,i,j-1}^+ E_{i,j-1}^l + \xi_{y\,i,j}^+ E_{i,j}^l + \zeta_{y\,i,j+1}^+ E_{i,j+1}^l \end{aligned} \quad (12)$$

$$\begin{aligned} & \zeta_{y\,i,j-1}^- E_{i,j-1}^{l+1} + \xi_{y\,i,j}^- E_{i,j}^{l+1} + \zeta_{y\,i,j+1}^- E_{i,j+1}^{l+1} \\ & = \zeta_{x\,i-1,j}^+ E_{i-1,j}^{l+1/2} + \xi_{x\,i,j}^+ E_{i,j}^{l+1/2} + \zeta_{x\,i+1,j}^+ E_{i+1,j}^{l+1/2} \end{aligned} \quad (13)$$

in which

$$\begin{aligned} \zeta_{\alpha\,i,j}^{\pm} &= \frac{jk n_0}{6} \pm \frac{\Delta z}{2\Delta\alpha^2} \pm \frac{\nu_{i,j}\Delta z}{48}, \\ \xi_{\alpha\,i,j}^{\pm} &= \frac{5jk n_0}{3} \mp \frac{\Delta z}{\Delta\alpha^2} \pm \frac{5\nu_{i,j}\Delta z}{24} \end{aligned}$$

where $\alpha = x$ or y .

At the edge of the computational window the transparent boundary condition (TBC) [22] is imposed. The TBC may fail for radiation fields with an appreciable wave vector spread. However, as will be shown later, the TBC works well in the analysis of a bent waveguide. This is due to the fact that the radiation field is dominated by a single transverse wave vector component.

To demonstrate the effectiveness of the GD scheme, we first investigate the propagation error of the fundamental mode LP₀₁ in a step-index optical fiber. We evaluate the following mode-mismatch loss L_M

$$L_M = -10 \log \left(\left| \int E_0 E^* dx dy \right|^2 / \left[\int |E_0|^2 dx dy \right]^2 \right) [\text{dB}] \quad (14)$$

where E is the propagating field and E_0 is the incident field of the fundamental mode. The mode-mismatch loss is known to be a sensitive indicator of the accuracy of a beam-propagation method [3].

The fiber has a core radius of $r = 5 \mu\text{m}$, and the refractive indices of $N_{CO} = 1.504$ and $N_{CL} = 1.500$. A stepped approximation is used for the circular core [18]. The computational window dimensions are given by $L_x \times L_y = 125 \times 125 \mu\text{m}^2$ and the wavelength is $\lambda = 1.55 \mu\text{m}$. In the analysis, the reference index is chosen to be that in the cladding.

Fig. 1 shows the mode-mismatch loss evaluated at $z = 500 \mu\text{m}$ as a function of propagation step length Δz . For comparison, the data obtained from the conventional ADIM based on the CN scheme are also presented. It is found that the accuracy of the GD scheme is better than that of the CN scheme. The numerical result is not a sensitive function of Δz .

III. SEMIVECTORIAL FORMULATION

Consideration is next given to the semivectorial analysis, in which we solve the scalar wave equation but accounts for the discontinuity in fields caused by the index variation. The semivectorial Fresnel equation is expressed as

$$\sigma \frac{\partial E}{\partial z} = \frac{\partial}{\partial x} \left(\frac{1}{n^2} \left\{ \frac{\partial}{\partial x} (n^2 E) \right\} \right) + \frac{\partial^2 E}{\partial y^2} + \nu E. \quad (15)$$

Equation (15) can also be solved by the ADIM. Equations corresponding to (10) and (11) are, respectively

$$\left(\sigma \frac{\partial E}{\partial z} \right)^l = 2 \left(\frac{\partial^2 E}{\partial y^2} \right)^l + \nu E^l \quad (16)$$

$$\left(\sigma \frac{\partial E}{\partial z} \right)^{l+1/2} = 2 \frac{\partial}{\partial x} \left(\frac{1}{n^2} \left\{ \frac{\partial}{\partial x} (n^2 E) \right\} \right)^{l+1/2} + \nu E^{l+1/2}. \quad (17)$$

The second derivative with respect to y can be treated as in the case of (3). Unfortunately, the Taylor's series expansion regarding the second derivative with respect to x is not simple because of the existence of the index term. Therefore, by analogy with (2) we assume the following relation based on the Stern's expression [23]

$$\begin{aligned} \frac{\partial}{\partial x} \left(\frac{1}{n^2} \left\{ \frac{\partial}{\partial x} (n^2 E) \right\} \right) &= \frac{a_i E_{i-1} - 2b_i E_i + c_i E_{i+1}}{\Delta x^2} \\ &\quad - \frac{1}{12} \delta^2 \left(\sigma \frac{\partial E}{\partial z} - \nu E \right) \end{aligned} \quad (18)$$

in which

$$\begin{aligned} a_i &= \frac{2n_{i-1}^2}{n_{i-1}^2 + n_i^2}, \\ b_i &= n_i^2 \left(\frac{1}{n_{i-1}^2 + n_i^2} + \frac{1}{n_i^2 + n_{i+1}^2} \right), \\ c_i &= \frac{2n_{i+1}^2}{n_{i+1}^2 + n_i^2}. \end{aligned}$$

Although (18) does not ensure the truncation error of $O(\Delta x)^4$, it leads to substantial improvement in accuracy as will be found later.

After some manipulations, we obtain the following difference equations:

$$\begin{aligned} & \zeta_{x\,i-1,j}^- E_{i-1,j}^{l+1/2} + \xi_{x\,i,j}^- E_{i,j}^{l+1/2} + \eta_{x\,i+1,j}^- E_{i+1,j}^{l+1/2} \\ & = \zeta_{y\,i,j-1}^+ E_{i,j-1}^l + \xi_{y\,i,j}^+ E_{i,j}^l + \zeta_{y\,i,j+1}^+ E_{i,j+1}^l \end{aligned} \quad (19)$$

$$\begin{aligned} & \zeta_{y\,i,j-1}^- E_{i,j-1}^{l+1} + \xi_{y\,i,j}^- E_{i,j}^{l+1} + \zeta_{y\,i,j+1}^- E_{i,j+1}^{l+1} \\ & = \zeta_{x\,i-1,j}^+ E_{i-1,j}^{l+1/2} + \xi_{x\,i,j}^+ E_{i,j}^{l+1/2} + \eta_{x\,i+1,j}^+ E_{i+1,j}^{l+1/2} \end{aligned} \quad (20)$$

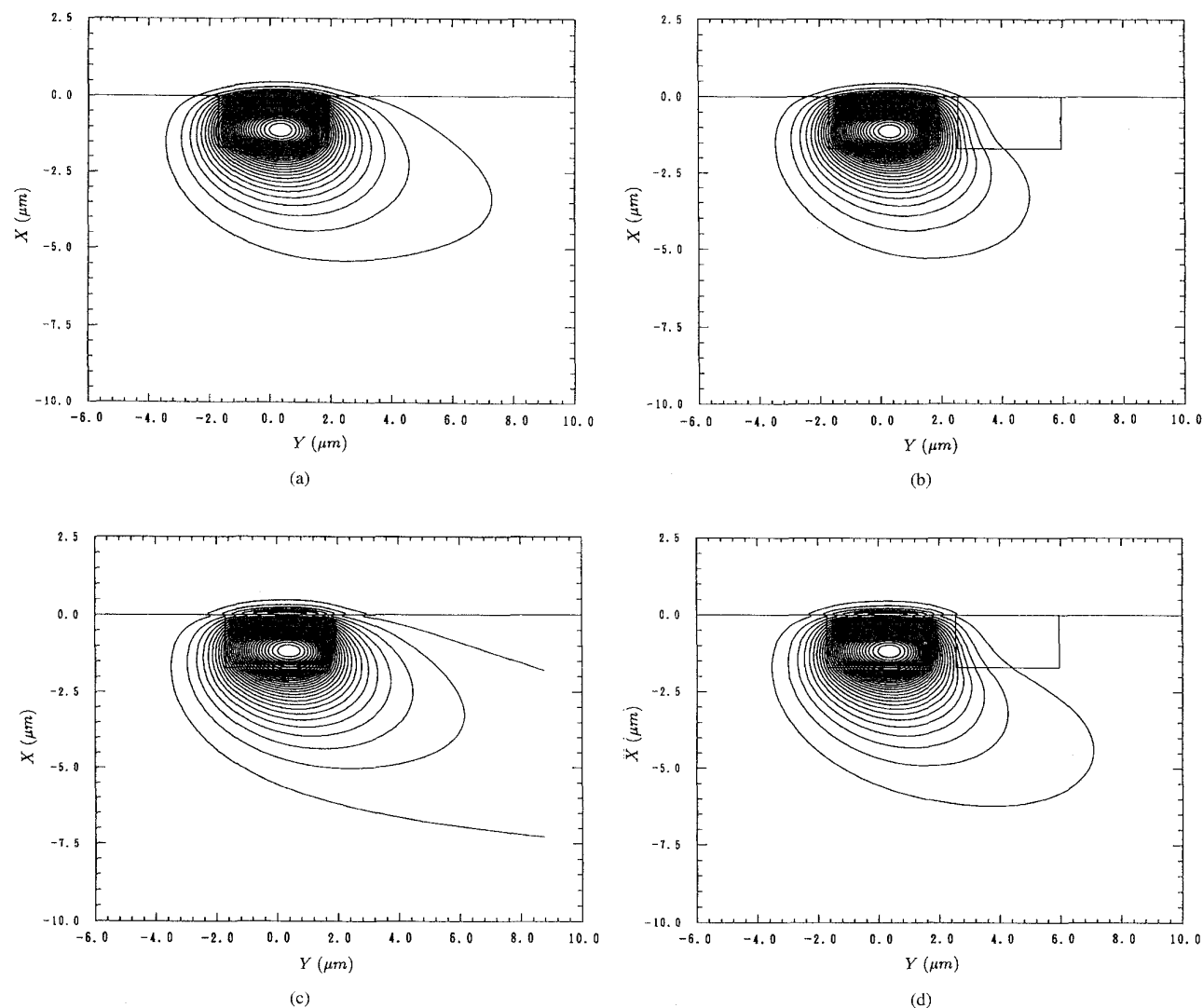


Fig. 4. Field distributions of a bent embedded optical waveguide. (a) Quasi-TE mode without trench, (b) quasi-TE mode with trench, (c) quasi-TM mode without trench, and (d) quasi-TM mode with trench.

in which

$$\begin{aligned}\zeta_{x i, j}^{\pm} &= \frac{jkn_0}{6} \pm \frac{\Delta z}{2\Delta x^2} a_{i, j} \pm \frac{\nu_{i, j} \Delta z}{48} \\ \xi_{x i, j}^{\pm} &= \frac{5jkn_0}{3} \mp \frac{\Delta z}{\Delta x^2} b_{i, j} \pm \frac{5\nu_{i, j} \Delta z}{24} \\ \eta_{x i, j}^{\pm} &= \frac{jkn_0}{6} \pm \frac{\Delta z}{2\Delta x^2} c_{i, j} \pm \frac{\nu_{i, j} \Delta z}{48} \\ \zeta_{y i, j}^{\pm} &= \frac{jkn_0}{6} \pm \frac{\Delta z}{2\Delta y^2} \pm \frac{\nu_{i, j} \Delta z}{48} \\ \xi_{y i, j}^{\pm} &= \frac{5jkn_0}{3} \mp \frac{\Delta z}{\Delta y^2} \pm \frac{5\nu_{i, j} \Delta z}{24}.\end{aligned}$$

To verify the improvement in the numerical accuracy of the semivectorial analysis, we treat two step-index slab waveguides with a different core index N_{CO} . The propagation of TM_0 mode is studied together with that of TE_0 mode. The core width is designated as $2D$. The normalized frequency is taken to be $V = 1.5$. The cladding index N_{CL} is fixed to be

1.0. The computational window dimensions are $6.10 \mu\text{m}$ and $14.88 \mu\text{m}$ for $N_{CO} = 1.5$ and 1.1 , respectively. This means that the number of transverse sampling points is in a range of 200 to 600 depending on Δx under the condition of the fixed window dimension. The wavelength is $\lambda = 1 \mu\text{m}$. The loss evaluation is carried out at a propagation distance of $500 \mu\text{m}$.

Fig. 2 shows the mode-mismatch loss as a function of transverse sampling width. For comparison, the results obtained by the CN scheme are also shown. The mode-mismatch loss observed for the GD scheme is found to be much smaller than that for the CN scheme. It is worth mentioning that the GD scheme is effective even in the TM mode.

As an application of the GD scheme to a three-dimensional waveguide, we analyze a bent embedded waveguide shown in Fig. 3. The refractive indexes are $N_{CO} = 1.55$ and $N_{CL} = 1.50$. The wavelength of $\lambda = 1.55 \mu\text{m}$ is used. The aspect ratio of W/T is chosen to be 2, and the width W is taken to be $3.4 \mu\text{m}$, so that only the fundamental mode propagates. The

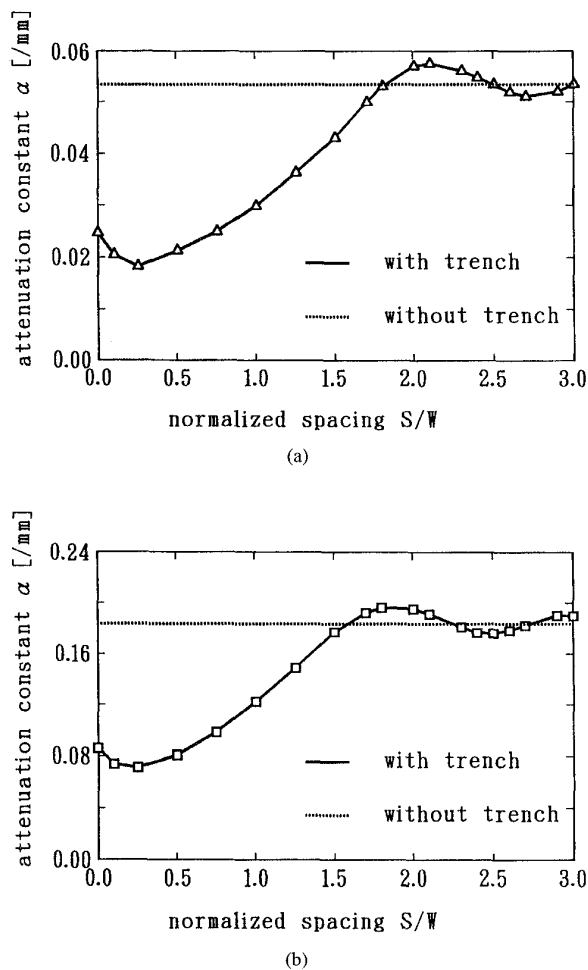


Fig. 5. Attenuation constant as a function of spacing between core and trench. (a) Quasi-TE mode and (b) quasi-TM mode.

bending radius is $R = 500 \mu\text{m}$. The computation parameters are as follows; $\Delta x = \Delta y/2 = 0.085 \mu\text{m}$, $\Delta z = 0.25 \mu\text{m}$, the numbers of transverse sampling points are $N_x = 120$ and $N_y = 160$. The fundamental-mode field is excited at $z = 0$. The index profile of the waveguide bend is transformed into that of an equivalent straight waveguide [24].

Fig. 4(a) and (c) shows the steady-state field distribution observed at a propagation distance of $1200 \mu\text{m}$. It is seen that the field deforms toward the outer side of the bend. The deformation of the field for the quasi-TM mode is found to be larger than that for the quasi-TE mode. This results in a larger attenuation constant in the quasi-TM mode as will be shown in Fig. 5.

To suppress the field deformation, we place the trench section at the outer side of the bend, as shown in Fig. 3. The width of the trench is the same as that of the core. The refractive index in the trench is $N_{\text{TR}} = 1.45$, and the spacing between the core and the trench is $S = W/4$. Figures 4(b) and (d) show how the trench enhances the field evanescence.

Effects of the trench location on the attenuation constant α are shown in Fig. 5. The attenuation constant is evaluated

using

$$\alpha = -\frac{1}{2\Delta z} \ln\left(\frac{P(z + \Delta z)}{P(z)}\right). \quad (21)$$

The ADIM with the phase term being not split does not conserve power. Therefore, we should check that α evaluated for the straight waveguide is sufficiently smaller than that caused by the bend. Preliminary calculation shows that α for the straight waveguide is less than $0.00004/\text{mm}$ for both modes, and is negligible in the following discussion.

Fig. 5 shows that the attenuation constant is small when the trench is made near the core. The appropriate location of the trench is close to the so-called radiation point, where the field becomes radiative. In this case, the appropriate location is around $S = W/4$ regardless of the polarization. It is also seen that α exhibits oscillatory behavior as a function of spacing S , as in the case of a two-dimensional step-index slab waveguide [19]. As discussed in detail in [20], this behavior can be explained by the fact that the sandwiched region between the core and the trench turns to a quasiwaveguiding region whose effective index changes as a function of spacing S . As expected, α converges to a value without the trench as the spacing S is further increased.

IV. CONCLUSION

The improved FD-BPM based on the generalized Douglas scheme for variable coefficients, in which the phase term is not split, has been discussed. The use of the Peaceman-Rachford ADIM achieves the reduced truncation error in the transverse directions, maintaining a tridiagonal system of linear equations. The computational time is almost identical to that in the conventional CN scheme. The mode-mismatch loss calculation shows that the present scheme is effective even in the analysis of TM mode propagation. As an example of the semivectorial analysis, the field deformation and the attenuation constant of a bent embedded waveguide are evaluated. Calculation shows how the trench enhances the field evanescence with subsequent reduction in the attenuation constant.

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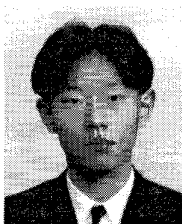
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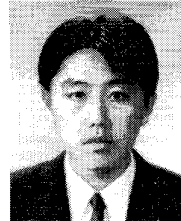
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