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Topology Optimization of Optical Waveguide Devices Based on Beam Propagation Method With Sensitivity Analysis

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Abstract—We present a gradient-based topology optimization method of optical waveguide devices using the beam propagation method (BPM). Efficient topology optimization of an optical waveguide is available by using our approach because it utilizes the adjoint variable method (AVM) for sensitivity analysis, and the BPM for numerical propagation analysis. In this paper, a way of evaluating sensitivities for a design of longitudinally varying waveguides is newly described in the case that a density method and finite difference BPM (FD-BPM) are employed. In addition, the validity and availability of our proposed method are verified by optimizing an S-bend and a Y-branch waveguides.

Index Terms—Topology optimization, Adjoint variable method, Beam propagation method, Optical waveguide device.

I. INTRODUCTION

In recent years, high speed and large capacity communication systems are required. High performance optical waveguide devices are in demand to realize these systems. Recently, the optimal design of optical waveguide devices based on the topology optimization method has attracted lots of attention. Compared with size or shape optimization, the advantage of the topology optimization method is that it has a great flexibility. Therefore, there is a potential for designing the unconventional and high performance devices by using the topology optimization.

Topology optimization method has already been applied to design optical waveguide devices such as photonic crystal waveguide devices [1]– [6]. We also have reported the application to optical waveguides and confirmed the validity of topology optimization [7]– [11]. Although the finite element method (FEM) or finite difference time domain (FDTD) method are used as a propagation analysis method in these reports, topology optimization does not restrict a numerical calculation method to the FEM or FDTD. Thus one can select a suitable wave propagation analysis method depending on a design problem in topology optimization.

Beam propagation method (BPM) is a quite useful technique in the case that backward wave reflections are negligible and refractive index varies slowly along the propagation direction. The wavefront matching (WFM) method [12], [13], which utilizes a principle of the BPM, is proposed as an optimal design method of weakly guiding optical waveguides. An optimum refractive index distribution can be synthesized automatically using the WFM. Several applications using the WFM method has been reported, for instance, a Y-branch waveguide [14], a crossing waveguide [15], and an arrayed-waveguide grating [16] for integrated planar lightwave circuits. The optimal design technique in [12] has a disadvantage in that a complicated refractive index distribution which is called “mosaic-like pattern” is appeared. This drawback is to some extent overcome by using “Solid pattern” approach proposed in [13]. However, WFM is not based on an objective function minimization problem, and the arbitrariness of objective property has not been discussed yet.

Topology optimal design problem is able to be efficiently solved by using a gradient method like a steepest descent if sensitivities for the design parameters are easily evaluated. Sensitivities of enormous design parameters have to be calculated in gradient-based topology optimization. In the topology optimization process, it is not practical to approximate a lot of sensitivities by finite difference scheme, therefore, an adjoint variable method (AVM) can be utilized for analyzing the sensitivities efficiently. A size optimization of optical waveguides using the AVM and BPM has already been proposed [17], [18]. However, topology optimization based on these approaches has not yet been discussed.

In this paper, we describe a topology optimal design method using the AVM and finite difference BPM (FD-BPM). A general way of evaluating sensitivities with a central AVM (CAVM) and the BPM has been described in [17], [18] for the optimization of the size or refractive index. In our approach, a density method, which is widely used in the topology optimization, is used as a representation of refractive index distribution and we describe a way to evaluate sensitivities for a longitudinally varying waveguide without using CAVM in the case that the density method is employed. By using our approach, an optical waveguide device can be designed using the topology optimization even if the device is too long to be analyzed with reasonable computer resources by the FEM or FDTD. We confirm the validity of our proposed topology optimal approach by applying it to a design of an S-bend and a Y-branch waveguides.

In Section II, we firstly review the formulation of FD-BPM, then a way of a representation of the refractive index distribution is described. Moreover, sensitivity analysis method
in the case of using the FD-BPM and the density method is described in Section III. After that, the design examples of the application of our approach are shown in Section IV. Finally, we state the conclusion in Section V.

II. TOPOLOGY OPTIMIZATION

A. Formulation of the FD-BPM

Now we consider a two dimensional planar optical waveguide, as shown in Fig. 1. In isotropic, linear and non-dispersive dielectric media, 2-D scalar Helmholtz equation for TE and TM polarized waves is given as follows:

\[
\frac{\partial}{\partial x} \left( p \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial z} \left( p \frac{\partial \Phi}{\partial z} \right) + k_0^2 n^2 \Phi = 0,
\]

where \( k_0 \) is a free-space wavenumber, \( n(x, z) \) is a refractive index distribution. By assuming \( \partial n/\partial z \approx 0 \) and \( \Phi(x, z) = \phi(x, z) \exp(-jk_0 n_0 z) \), the following basic BPM equation is obtained,

\[
\frac{\partial^2 \phi}{\partial z^2} + j2k_0 n_0 \frac{\partial \phi}{\partial z} = (D_{xx} + \nu) \phi,
\]

with

\[
D_{xx} = \frac{1}{p} \frac{\partial}{\partial x} \left( p \frac{\partial}{\partial x} \right), \\
\nu = k_0^2 (n^2 - n_0^2),
\]

where \( n_0 \) is a reference refractive index. In the paraxial BPM equation, \( \partial^2 \phi/\partial z^2 \) is omitted. Then, the following sequential update equation of the BPM can be obtained by using implicit FD scheme for Eq. (2) [19],

\[
[A]_i \{ \phi \}_{i+1} = [B]_i \{ \phi \}_i,
\]

where \([A]_i\) and \([B]_i\) are the matrices obtained by spatial discretization, \( i(= 0, 1, 2, \ldots, N_z - 1) \) is the step number of the \( z \)-direction.

In this paper, we employ the paraxial approximation on the basic BPM equation. In addition, the transverse direction is discretized by using a FD scheme proposed by Stern [20]. The transparent boundary condition [21] is employed as an absorbing boundary condition.

B. Representation of refractive index distribution

In the topology optimization, the representation of refractive index distribution is one of the most important issues. Here, we employ the density method to describe the refractive index in design region. The refractive index distribution is represented by the normalized density distribution \( \rho(x, z) \) [1]. A drawback of conventional density method is that a gray region, in which \( 0 < \rho < 1 \), appears. In order to suppress the gray regions, we express the refractive index distribution by using a Heaviside filter \( H(\rho) \) as follows:

\[
n^2(x, z) = n_1^2 + (n_2^2 - n_1^2)H(\rho),
\]

\[
H(\rho) = \begin{cases} 
0.5(2\rho)^m & (0 \leq \rho < 0.5) \\
1 - 0.5(2 - 2\rho)^m & (0.5 \leq \rho \leq 1)
\end{cases}
\]

where \( m \) is a penalty parameter, \( n_1 \) and \( n_2 \) are the refractive indices of the core and cladding region, respectively. In the practical optimization, the density distribution is discretized on the finite difference grids. As shown in Fig. 2, \( H(\rho) \) is a step-like function approximately if \( m \) is a large value. Thus, a binarized refractive index distribution is obtained by \( m \to \infty \). However, \( n(x, z) \) has to be differentiated by the density parameter in the sensitivity analysis, thus the topology is not freely modified in the case that the value of \( n \) is raised excessively. Therefore, in this paper, \( m \) is taken to be a lower value in the initial phase of the optimization. Then, the value of \( m \) is raised as iterating the optimization, finally, \( m \) is set to infinity.

III. SENSITIVITY ANALYSIS

Now we describe the sensitivity analysis method in the case of using the 2-D BPM and the density method. We assume the design parameters are allocated for each discrete point in the design region. A sensitivity of an objective function \( C \) is defined by \( \partial C/\partial \rho_{i,j} \) where \( \rho_{i,j} \) is a density parameter, \( j(= 0, 1, 2, \cdots, N_x - 1) \) is an index number along the \( x \)-direction. Properties of optical waveguides are usually represented by an S-parameter, i.e. \( S_{n1} \), where \( n \) is the output port number. Thus, we consider that \( C \) depends on the normalized power \( |S_{n1}|^2 \) in the port \( n \). The sensitivity of \( |S_{n1}|^2 \) is expressed by

\[
\frac{\partial |S_{n1}|^2}{\partial \rho_{i,j}} = \text{Re} \left\{ 2S_{n1}^* \frac{\partial S_{n1}}{\partial \rho_{i,j}} \right\},
\]
where * means complex conjugate. \( S_{n1} \) can be represented by the following overlap integral,

\[
S_{n1} = \int \psi_n^* \phi_N \, dx,
\]

(6)

where \( \psi_n \) is an eigenmode field in the port \( n \). In the case that FD scheme is employed, by using the rectangle rule, Eq. (6) can be rewritten as follows:

\[
S_{n1} = \Delta x \{ \psi_n \}^\dagger \{ \phi \}_{N_x},
\]

(7)

where \( \dagger \) means Hermitian transpose, \( \Delta x \) is a step width along the \( x \)-direction. By substituting Eq. (3) into Eq. (7), we can obtain

\[
S_{n1} = \Delta x \{ \psi_n \}^\dagger \{ [A]^{-1} [B] \}_{N_y-1} \{ [A]^{-1} [B] \}_{N_y-2} \cdots \{ [A]^{-1} [B] \}_1 \{ [A]^{-1} [B] \}_0 \{ \phi \}_0.
\]

(8)

By taking the derivative of \( S_{n1} \) with respect to a density parameter \( \rho_{i,j} \), we get

\[
\frac{\partial S_{n1}}{\partial \rho_{i,j}} = \Delta x \{ \psi_n \}_{i+1}^\dagger \left( -[A]^{-1} \frac{\partial [A]}{\partial \rho_{i,j}} \{ \phi \}_{i+1} + [A]^{-1} \frac{\partial [B]}{\partial \rho_{i,j}} \{ \phi \}_i \right),
\]

(9)

where

\[
\{ \psi_n \}_{i+1}^\dagger = \{ \psi_n \}^\dagger \{ [A]^{-1} [B] \}_{N_y-1} \{ [A]^{-1} [B] \}_{N_y-2} \cdots \{ [A]^{-1} [B] \}_1 \{ [A]^{-1} [B] \}_0.
\]

(10)

Here, \( \{ \psi_n \}_{i+1} \) is a backward propagating field of \( \{ \psi_n \} \) which comes from the output port \( n \). Figure 3 shows the sensitivity analysis using the BPM. \( \{ \phi \}_j \), \( \{ \phi \}_{i+1} \), and \( \{ \psi_n \}_{i+1} \) in Eq. (9) are obtained by the forward and backward beam propagations. The refractive index distribution is represented by Eq. (4), thus \( \partial [A]_i / \partial \rho_{i,j} \) and \( \partial [B]_i / \partial \rho_{i,j} \) can be calculated analytically without using CAVM. After calculating forward and backward wave propagation fields, the sensitivities for all design parameters can be evaluated by simple matrix-vector products. Therefore, efficient topology optimization can be achieved by using this approach.

IV. DESIGN EXAMPLES

In this section, in order to demonstrate the validity of our approach, we consider two design examples of weakly guiding optical waveguides. In these examples, a steepest descent method is employed to minimize an objective function. The design parameters are updated by following equation:

\[
\rho_{i,j}^{M+1} = \rho_{i,j}^M - \frac{1}{K} \frac{\partial C}{\partial \rho_{i,j}},
\]

(11)

where \( M \) is an iteration number, \( K \) is a constant which is taken to be as follows:

\[
K = \max_{i,j \in \Omega} \left| \frac{\partial C}{\partial \rho_{i,j}} \right|.
\]

(12)

where \( \Omega \) represents a set of discrete points in the design region. After updating the density parameters, \( \rho_{i,j} \) is reset to \( 0 + \delta \) or \( 1 - \delta \) in the case of \( \rho_{i,j} \leq \delta \) or \( 1 - \delta \leq \rho_{i,j} \), respectively, where \( \delta \) is an arbitrarily small value and is introduced for avoiding the sensitivity to be zero. In this paper, we select \( \delta \) to be \( 10^{-6} \). The above constants, \( K \), \( \delta \), of course, have to be changed properly depending on a design problem.

A. S-bend waveguide

Now we design a 2-D S-bend waveguide whose design model is shown in Fig. 4. We assume a fundamental TE mode (TE₀ mode) at the wavelength of 1.55 \( \mu m \) is launched into port 1. The core and cladding refractive indices are \( n_1 = 1.45 \) and \( n_2 = 1.445 \), respectively. The configuration parameters of the design model are as follows: \( w = 5 \, \mu m \), \( L = 800 \, \mu m \),
normalized output power

\[
\begin{array}{cccc}
0.84 & 0.86 & 0.88 & 0.92 \\
0.94 & 0.96 & 0.98 & 1.00 \\
1.00 & 0.90 & 0.90 & 1.50 \\
1.50 & 1.60 & 1.65 & 1.70
\end{array}
\]

\text{Normalized output power}

\text{Wavelength [\mu m]}

\text{(a) Optimized refractive index distribution}
\text{(b) Field pattern([E_y])}

Fig. 6. The refractive index distribution and the field pattern of the optimized S-bend waveguide.

\text{(a) Optimized refractive index distribution}
\text{(b) Field pattern([E_y])}

Fig. 7. The refractive index distribution and the field pattern of the optimized S-bend waveguide using a smoothing filter.

\[d = 30 \, \mu m, \, l = 100 \, \mu m, \, \text{and} \, D = 40 \, \mu m\].

The input and output waveguides are configured to be operated as a single mode waveguide at the wavelength of 1.55 \mu m. To maximize the output power of TE\(_0\) mode, we define the objective function as follows:

\[
\text{Minimize } C = \left[1 - |S_{21}|^2\right]^2.
\]

The reference index \(n_0\) is taken to be the effective index of TE\(_0\) mode in the input waveguide. The step widths are \(\Delta x = 0.2 \, \mu m\) and \(\Delta z = 1 \, \mu m\). The penalty parameter changes from \(m = 2\) to 64 linearly during the optimization process. We give an uniform refractive index distribution (\(\rho = 0.3\)) as an initial structure in the design region in order to show the special initial structure is not required. Unnecessary core refractive index regions appear in the optimized structure in the case that \(\rho \geq 0.5\) in the initial uniform region. In addition, too small value of \(\rho\) leads to a nearly zero sensitivity, thus the device performance is not efficiently improved in this optimization process.

The normalized output power as a function of the number of iterations is shown by the solid curve in Fig. 5. We can see that the transmission property is improved with the iteration. The optimized refractive index distribution of the S-bend waveguide and its field pattern are shown in Fig. 6. Offsets of the waveguide for mode matching at the input and output ports, and the grating-like structures emerge to suppress the radiation waves in the optimized distribution. The normalized output power in the binarized optimized refractive index distribution is 0.941. Considering practical production, it is preferable that a fine structure does not emerge. The dashed curve shown in Fig. 5 is the normalized output power as a function of the number of iterations in the case of using a smoothing filter which is a simple moving average filter with \(3 \times 3\) kernel size. The discretized density parameter distribution \(\rho_{i,j}\) is filtered at each iteration as follows:

\[
\rho_{i,j}^{\text{filtered}} = \sum_{\xi=-1}^{1} \sum_{\eta=-1}^{1} \frac{1}{9} \rho_{i+\xi,j+\eta}.
\]

Although the output power vibrates marginally in consequence of the smoothing filter, the transmission property in the optimized S-bend is almost the same with the previous results. The optimized refractive index distribution and its field pattern using the smoothing filter are shown in Fig. 7. Compared with Fig. 6(a), we can see that a simpler refractive index distribution is obtained. The normalized output power in the binarized optimized refractive index distribution is 0.955 when the smoothing filter is employed.

Figure 8 shows the wavelength dependence of the normalized output power of optimized S-bend waveguides. Although the grating-like structure emerges in optimized S-bend waveguide, broadband property is obtained especially in the case of using the smoothing filter. The designed structure shown in Fig. 7(a) is required to be insensitive to the slight structural deviation induced by the smoothing filter. Consequently, using smoothing filter seems to lead to the optimized structure whose transmission property is insensitive to wavelength.

\[B. \, Y\text{-branch waveguide}\]

In this subsection, we consider a weakly guiding 2-D Y-branch waveguide which divides the input power equally into two ports in this example. The design model of a Y-branch waveguide is shown in Fig. 9. The configuration parameters of the design model are as follows: \(w = 5 \, \mu m\), \(L = 500 \, \mu m\), \(d_1 = 50 \, \mu m\), \(d_2 = 30 \, \mu m\), \(l = 50 \, \mu m\), and \(D = 40 \, \mu m\). In order to equally divide the power into port 2 and 3, we set the objective function as follows:

\[
\text{Minimize } C = \left[\frac{1}{2} - |S_{21}|^2\right]^2 + \left[\frac{1}{2} - |S_{31}|^2\right]^2.
\]

In addition, we impose a symmetry condition to keep the power division equally into port 2 and 3. The other design conditions are same as the previous design example.
The normalized output power in port 2 and 3 as a function of the number of iterations are shown in Fig. 10. In this design example also, the transmission characteristics are improved with the iteration. The normalized output power with the binarized optimized refractive index distribution is 0.490 in each port. The optimized refractive index distribution of the Y-branch waveguide and the field pattern are shown in Fig. 11. In the vicinity of the input port, the structure which can reduce the radiation into the longitudinal direction emerges. Y-branch profile similar to this structure was proposed, for instance in [22]. Moreover, as is the case in the design of the S-bend waveguide, offsets in the both output ports and the grating-like structure emerge in the optimized structure.

Our approach is based on an objective function minimization problem. Thus, for instance, $(X : Y)$ power divider can be designed by setting the objective function as follows:

$$\text{Minimize } C = W_1 C_1 + W_2 C_2,$$

$$C_1 = \left| Y S_{31} \right|^2 - \left| Y S_{21} \right|^2,$$

$$C_2 = \left| 1 - \left( \left| S_{21} \right|^2 + \left| S_{31} \right|^2 \right) \right|^2,$$

where $W_1$ and $W_2$ are the weighting parameters and are taken to be,

$$W_1 = \frac{C_1}{C_1 + C_2}, \quad W_2 = \frac{C_2}{C_1 + C_2}.$$

Due to the weighting parameters, larger one of them, $C_1$ and $C_2$, is minimized preferentially.

Using the optimized Y-branch structure as the initial refractive index distribution shown in Fig. 11(a) and the smoothing filter, we design three power dividers which have different splitting ratios. The structure of optimized $(X : Y)$ power divider and its field patterns are shown in Fig. 12. The insertion loss and the splitting ratio of each optimized structure at a wavelength of 1.55 μm and the wavelength dependence are shown in Table I and Fig. 13, respectively. We can see that a low wavelength dependence is realized in the optimized power dividers owing to using the smoothing filter although larger splitting ratio causes larger insertion loss and greater wavelength dependence of the splitting ratio. As described in [9], an objective function taking account of the wavelength dependence should be used if a desired broadband property cannot be obtained. As shown in these design examples, an optical waveguide device which is hard to design based on theoretical approach can be found out automatically by using our approach.

| Table I | THE INSERTION LOSS AND THE SPLITTING RATIO OF THE OPTIMIZED $(X : Y)$ POWER DIVIDER. |
| --- | --- | --- |
| (3:2) power divider | -14.3 | 1.50 |
| (2:1) power divider | -16.0 | 2.00 |
| (3:1) power divider | -11.9 | 2.92 |

V. CONCLUSION

We presented a new approach of topology optimization of optical waveguides using the AVM and the BPM, and described the way to evaluate the sensitivities in the case of using the density method. We are the first to apply the topology optimization utilizing the BPM and the AVM to the design of weakly guiding waveguide devices.

We demonstrated that the low loss S-bend and Y-branch are found out by using our approach, therefore the validity of our approach is confirmed. Arbitrary transmission properties are configurable in our approach thus it can be applied to a design of an arbitrary waveguide device which has another function, such as a X-junction, a mode/wavelength/polarization...
In the case of utilizing topology optimization, arbitrary refractive index distribution can be appeared in the design region. The optimized devices shown in this paper are weakly guiding and these distributions do not violate the assumption of the BPM. However, in particular strongly guiding optical waveguides, the assumption may be violated. Topology optimization based on the FEM or FDTD has been successfully applied to strongly guiding waveguide problems [1]- [6], [9]-[11]. Thus, the applicability of our approach is principally limited by the assumption. It is known that the accuracy of the BPM is degraded at an abrupt refractive index change area. Therefore, our approach could be applied to the design of strongly guiding optical waveguides by developing some additional constraint condition to suppress an emergence of the abrupt refractive index change. It is also our future work.

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