# A Study on Topology Optimization of Optical Circuits Consisting of Multi-Materials

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Kota Fujimoto, Yasuhide Tsuji, Member, IEEE, Koichi Hirayama, Senior Member, IEEE, Takashi Yasui, Member, IEEE, Shingo Sato, Member, IEEE, and Ryosuke Kijima

*Abstract*—A topology optimization method can be used to find out the optical waveguide structures which have the desired transmission characteristics. Using the function expansion method, we can avoid the problem of a gray area, which means that some areas having intermediate refractive index between those of usable materials appear in a design region. However, so far, topology optimization has mainly been studied for structures consisting of two isotropic materials. In this paper, we study the applicability of topology optimization to structures which include three or more materials, and demonstrate the optimal design of a waveguide crossing.

*Index Terms*—Topology optimization method, optical waveguide circuit, finite element method.

## I. Introduction

ALONG with a recent increase in communication traffic, the demand for high speed and flexible photonic network has been increasing. In order to realize the high speed and large-capacity photonic network, high-performance optical circuit devices are required to be used in the photonic network system. The design of optical devices using computer simulation is known to be effective. Furthermore, recently, a lot of researches on automatic generation of optimum optical device structures which can realize the desired properties have been reported. Optimization methods using numerical simulation techniques, such as genetic algorithms [1], [2], wavefront matching method [3], [4], and topology optimization [5]–[10], have been reported. Sizing optimization has also been reported for the optimal design of optical devices, for example in [11], where for a spot-size converter of a segmented waveguide, widths of the segments were optimized using an evolutionary algorithm. An optimization method which optimizes the refractive index distribution in a design region may require more computational time than a sizing optimization method, but we may find out a novel and more compact structure than an optimum one obtained using sizing optimization, in which the shape in a design region is fixed except for size throughout the optimization process. In this study, we consider the topology optimization based on the function expansion method that can avoid the fundamental problem of a gray area, which

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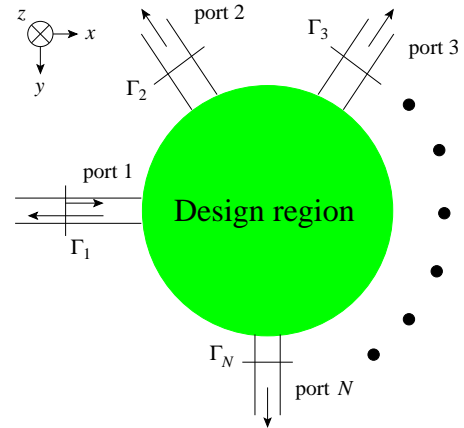


Fig. 1. Setup of optimization problem.

has intermediate refractive index between those of usable materials, and can design several devices.

In topology optimization, the optimal structure can be obtained by replacing the structure design optimization problem with the material distribution problem in the design region. The density method is widely used to represent the material distribution. However, the density method has the potential to cause an intermediate gray area that takes a value between 0 and 1 in optimizing the value of the density. In recent years, the topology optimization based on the function expansion method, which sets some function in a design region to determine the refractive index distribution, has been proposed [10]. In this approach, the refractive index at a certain point is set to be one of the two given values, which is chosen by comparison of the function value with a threshold value, so that no gray area appears. However, the discussion in [10] was limited to optimize the structures consisting of two isotropic materials. In this paper, the applicability of this approach to the optimization problems including three or more materials is examined and the optimal design of a waveguide crossing is demonstrated.

## II. Topology Optimization

### A. Representation of refractive index distribution in design region

Considering an optical waveguide device as shown in Fig. 1, and assuming the light is launched into the port 1, we consider the problem to optimize the refractive

index profile that can realize the desired transmission characteristics. In the topology optimization based on the function expansion method, the refractive index profile in the design region is expressed using a function with some unknown coefficients and those coefficients are iteratively updated so that the characteristics may be improved based on a sensitivity analysis. Now, if the device is designed using only two kinds of materials, dielectric constant can be defined as follows by using some analytical functions $w(x,y)$ [10]:

$$\varepsilon_r(x,y) = \varepsilon_{ra} + (\varepsilon_{rb} - \varepsilon_{ra})H(w(x,y)) \tag{1}$$

Here, $\varepsilon_{ra}$ and $\varepsilon_{rb}$ are the dielectric constants of the two considered materials. The function $H(w(x,y))$ takes the value of 0 or 1 depending on the value of $w(x,y)$ and $\varepsilon_r(x,y)$ at any points is the dielectric constant of either $\varepsilon_{ra}$ or $\varepsilon_{rb}$ depending on the value of $w(x,y)$. In order to make it possible to take differential of $H(w(x,y))$ in the sensitivity analysis described in Subsection II.C, we define $H(w(x,y))$ as follows:

$$H(w) = \begin{cases} 0 & (w \le -h) \\ \dfrac{1}{2}\left(\dfrac{w+h}{h}\right)^2 & (-h < w < 0) \\ 1 - \dfrac{1}{2}\left(\dfrac{w-h}{h}\right)^2 & (0 < w < h) \\ 1 & (w \ge h) \end{cases} \tag{2}$$

In this paper, in order to treat three or more materials in the optimization, (1) is extended to the following expression:

$$\varepsilon_r(x,y) = \varepsilon_{r,1} + \sum_{i=1}^{M}(\varepsilon_{r,i+1} - \varepsilon_{r,i})H(w(x,y) - t_i) \tag{3}$$

where $M$ is the number of materials considered in the optimization, $\varepsilon_{r,i}(i = 1, 2, \cdots M)$ are the dielectric constants of those materials, and $t_i$ is the threshold for each material. In the region where the function $w(x,y)$ takes the value between $t_i$ and $t_{i+1}$, the dielectric constant is defined to be $\varepsilon_{r,i+1}$.

Here, $w(x,y)$ is expressed in the form of the superposition of some analytical function $f_i(x,y)$ as

$$w(x,y) = \sum_{i=1}^{N} c_i f_i(x,y) \tag{4}$$

By optimizing the value of the coefficient $c_i$ based on sensitivity analysis, the optimal structure will be obtained. As the function $w(x,y)$, several kinds of functions can be used. In this paper, Fourier series represented by the following equation is used:

$$w(x,y) = \sum_{i=-N_x}^{N_x-1}\sum_{j=-N_y}^{N_y-1}(a_{ij}\cos\theta_{ij} + b_{ij}\sin\theta_{ij}) \tag{5}$$

$$\theta_{ij} = \frac{2\pi i}{L_x}x + \frac{2\pi j}{L_y}y \tag{6}$$

where $N_x$ and $N_y$ are the number of expansion terms in the $x$ and the $y$ directions, respectively. Fourier series is

intended to represent a periodic function. However, the addition of structural constraints of periodicity is not desirable. In order to remove such constraints, $L_x$ and $L_y$ have to be greater than the design region sizes along the $x$ and $y$ directions, respectively. (2) shows the dielectric constant takes intermediate values in $|w| < h$. However, gray area can be removed by setting $h$ to be 0 after the optimization process.

### B. Formulation by the Finite Element Method

In topology optimization, it is necessary to evaluate the characteristics of a given optical device. Here, we employ the finite element method (FEM) to evaluate the transmission characteristics.

We consider a two-dimensional optical waveguide structure as shown in Fig. 1, where boundary $\Gamma_n$ ($n = 1, 2, \cdots, N$) represents the port of the $n$-th waveguide. Dividing an analysis region into a number of second order triangular elements and applying FEM described in [12], we obtain a final matrix equation as follows:

$$[P]\{\Phi\} = \{u\} \tag{7}$$

with

$$\{u\} = [Q]\{\Psi\}_\Gamma \tag{8}$$

where $[P]$ and $[Q]$ are matrices generated by FEM, $\{u\}$ is a vector related to an incident wave on $\Gamma_1$, and $\Phi = E_z$ or $H_z$ ($E_z$ and $H_z$ being the $z$ component of electric and magnetic field, respectively) for TE or TM mode. These matrices and vectors are presented in detail in [12].

### C. Sensitivity Analysis

When using the function expansion method in the topology optimization, we need to know the dependence of the scattering parameter $S_{n1}$ on the expansion coefficient $c_i$ of (4). If Fourier series of (5) is employed as in this paper, $c_i$ in the formulation of this subsection should be interpreted as $a_{ij}$ and $b_{ij}$.

After solving the propagating field in the given optical waveguide devices by FEM and using the field vector on the $n$-th waveguide $\{\Phi_n\}$, the scattering parameter $S_{n1}$ can be written as follows:

$$S_{n1} = -\delta_{n1} + \frac{1}{A_1}\{g_n\}^T\{\Phi_n\} \tag{9}$$

with

$$\{g_n\}^T = \sqrt{\frac{\beta_n}{\beta_1}}\{\Psi_n\}^T[Q] \tag{10}$$

where $\{\Psi_n\}$ is the vector which consists of the values of $\Psi_n$ at the nodal points on the boundary $\Gamma_n$ and $\Psi_n$ is the mode profile of the fundamental mode of the $n$-th waveguide. Also, $\beta_n$ is the propagation constant of the fundamental mode of the $n$-th waveguide, $A_1$ is the amplitude of the incident fundamental mode at port 1, $\delta_{n1}$ represents the Kronecker delta, and $T$ denotes a transpose.
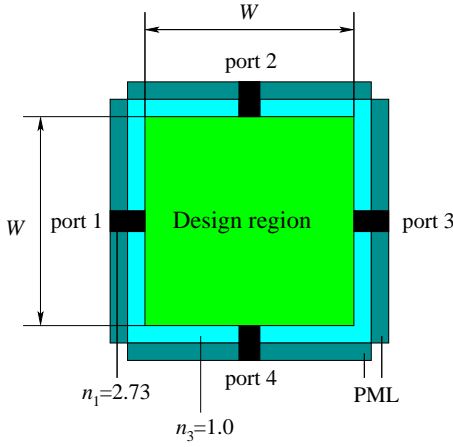
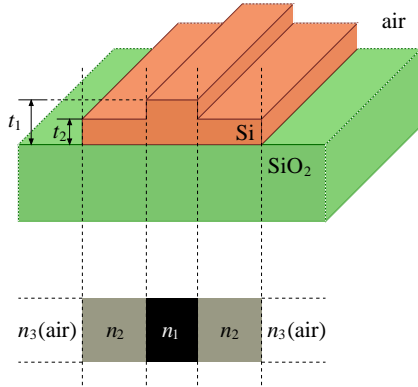Fig. 2.   Optimization model of waveguide crossing.



Fig. 3.   Equivalent index distribution of three dimensional waveguide.

To efficiently calculate the derivative of $S_{n1}$ with respect to $c_i$, adjoint variable method (AVM) can be used. First, we represent $\partial S_{n1}/\partial c_i$ as follows:

$$\frac{\partial S_{n1}}{\partial c_i} = \sum_k \frac{\partial S_{n1}}{\partial \Phi_k}\frac{\partial \Phi_k}{\partial c_i} = \left\{\frac{\partial S_{n1}}{\partial \Phi}\right\}^T \frac{\partial \{\Phi\}}{\partial c_i} \tag{11}$$

Here, the final equation of FEM is given in (7). Taking the derivative of (7) with respect to $c_i$, we obtain the following expression:

$$\frac{\partial [P]}{\partial c_i}\{\Phi\} + [P]\frac{\partial \{\Phi\}}{\partial c_i} = \{0\} \tag{12}$$

Substituting this equation to (11), we can get the following equation:

$$\frac{\partial S_{n1}}{\partial c_i} = -\{\lambda_n\}^T \frac{\partial [P]}{\partial c_i}\{\Phi\} \tag{13}$$

with

$$[P]^T\{\lambda_n\} = \left\{\frac{\partial S_{n1}}{\partial \Phi}\right\} \tag{14}$$

Once we can get $\{\lambda_n\}$ by solving (14), we can efficiently estimate $\partial S_{n1}/\partial c_i$ for all the $c_i$ by the product of the known vectors.
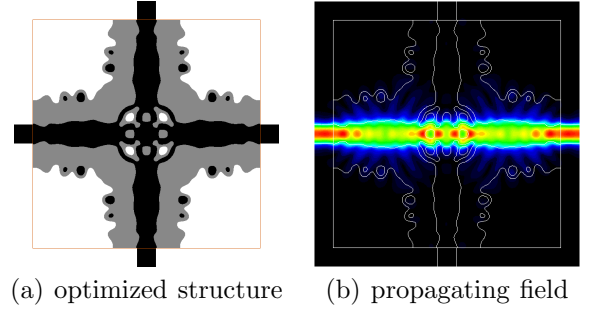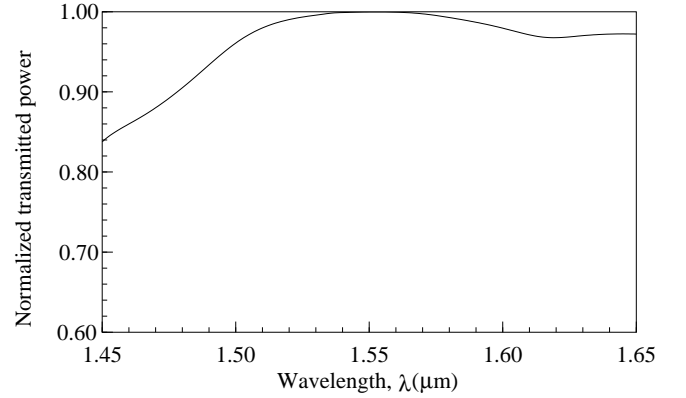


(a) optimized structure          (b) propagating field

Fig. 4.   Optimization results of waveguide crossing at wavelength of 1.55 $\mu$m.



Fig. 5.   Wavelength dependence of the normalized transmitted power of the optimized structure in the single-wavelength optimization.

### III. Optimal Design Example of an Optical Waveguide

In this section, we demonstrate the optimal design of optical waveguide devices using the optimization method described in the previous section. As an example of the topology optimization, we consider the waveguide crossing as shown in Fig. 2 and find out the device structure which can suppress the cross talk. In this problem, we consider the fundamental TE mode incidence and find out the structure in which the incident light into port 1 transmits into port 3 with minimized cross talk. In this optimization, we impose a symmetry condition in the $x$ and $y$ directions and also impose a 90 degree rotational symmetry condition. Therefore, if the incident light into port 1 can transmit to port 3 without any cross talk, the light into port 2 can also transmit to port 4 without any cross talk.

In this example, we assume that three materials can be used in the design region. The indices of these three materials are $n_1 = 2.73$, $n_2 = 2.1$, and $n_3 = 1.0$, where the materials of $n_1$ and $n_3$ are the same as the core and cladding of the waveguide. Since these three materials may be considered as equivalent materials with the effective index of the three-dimensional waveguide, as shown in Fig. 3, where the region with the different waveguide height is represented by the different effective index, it may be a case in which it is necessary to optimize structures including three materials. It is of much interest to

(a) initial structure    (b) $N_x = N_y = 4$

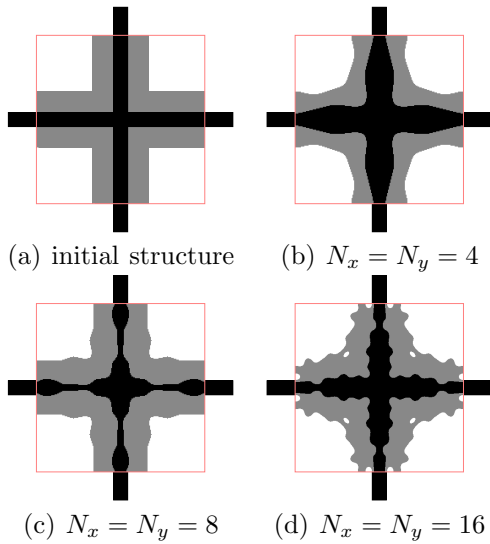(c) $N_x = N_y = 8$    (d) $N_x = N_y = 16$

Fig. 6. Initial structure of waveguide crossing and optimized ones for different numbers of expansion terms in the multi-wavelength optimization.
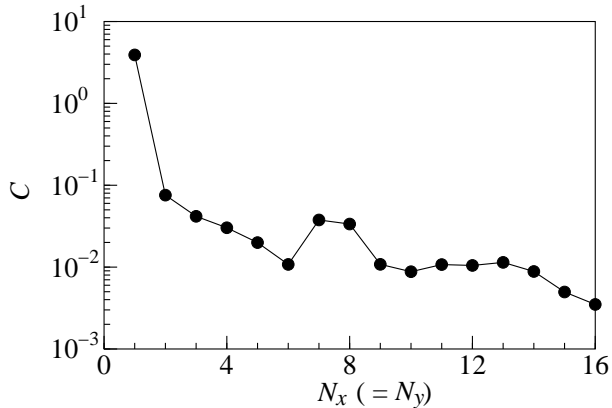


Fig. 7. Dependence of the minimized value of the objective function on the number of expansion terms in the multi-wavelength optimization.

investigate the optimization on three-dimensional optical waveguides, but that is beyond this paper. The purpose of this paper is to present topology optimization to structures including three or more materials, and we focus on the optimization of the two-dimensional waveguide crossing shown in Fig. 2. The waveguide width is $w = 0.5$ $\mu$m, the width of the design region is $W = 6$ $\mu$m, and the thickness of the PML is 0.5 $\mu$m to absorb the transmitted and radiated field.

First, we consider the optimization problem at a single wavelength $\lambda = 1.55$ $\mu$m and employ the following objective function to be minimized:

$$\text{Minimize } C = 1 - |S_{21}|^2 \qquad (15)$$

Fig. 4 shows the optimized structure and propagating field at $\lambda = 1.55$ $\mu$m. We can see that the incident light into port 1 transmits to port 3 with little cross talk. The obtained structure has a clear material boundary. However, the structure around the crossing region is a little
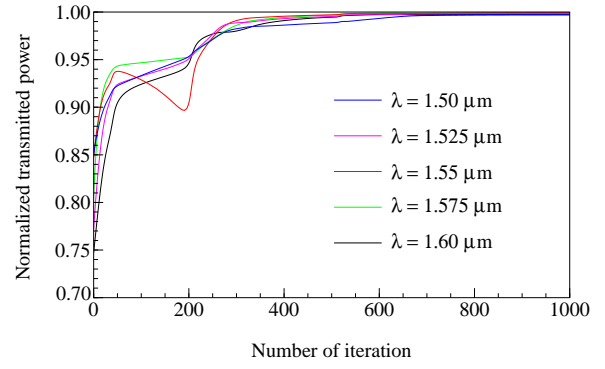


Fig. 8. Convergence behavior for optimization of waveguide crossing in the multi-wavelength optimization.

bit complicated. Fig. 5 shows the wavelength dependence of the transmission property. Because of the complicated structure around the crossing region, the relatively strong wavelength dependence is observed.

Next, in order to suppress the wavelength dependence, considering the 100 nm wavelength band width around 1.55 $\mu$m, we employ the following objective function to be minimized:

$$\text{Minimize } C = \sum_{i=1}^{K} (1 - |S_{21}(\lambda_i)|^2) \qquad (16)$$

where $K = 5$ and $\lambda_i$ for $i = 1, 2, 3, 4, 5$ is 1.5, 1.525, 1.55, 1.575, 1.6 $\mu$m, respectively.

We consider the initial structure as shown in Fig. 6(a), and the obtained optimized structures are shown in Figs. 6(b), (c), and (d) for $N_x = N_y = 4$, 8, and 16, respectively, where $N_x = N_y$ is assumed because of the symmetry of the waveguide crossing. In the single wavelength problem, there are several structures which can realize the desired property and the obtained structure in Fig. 4 is the one of those structures. In the multi-wavelength optimization, the structure originated at a specific wavelength is avoided and the simpler structures are obtained. Fig. 7 shows the dependence of the minimized value of the objective function on the number of expansion terms in the multi-wavelength optimization. We notice that the objective function is most minimized when $N_x = N_y = 16$, so we use $N_x = N_y = 16$ in the following computation.

The convergence behavior of the normalized transmitted power in the iteration process is shown in Fig. 8. The average transmitted power of five wavelengths increases in the iteration process, and finally the average transmitted power reaches 0.998. Fig. 9 shows the wavelength dependence of the normalized transmitted power of the non-optimized structure, i.e. the initial structure of Fig. 6(a), and optimized one. For comparison, the results for the non-optimized and optimized waveguide crossings with two materials, in which refractive indices of its core and cladding are, respectively, $n_1 = 2.73$ and $n_3 = 1.0$, are also shown in Fig. 9. We can see that the optimized waveguide
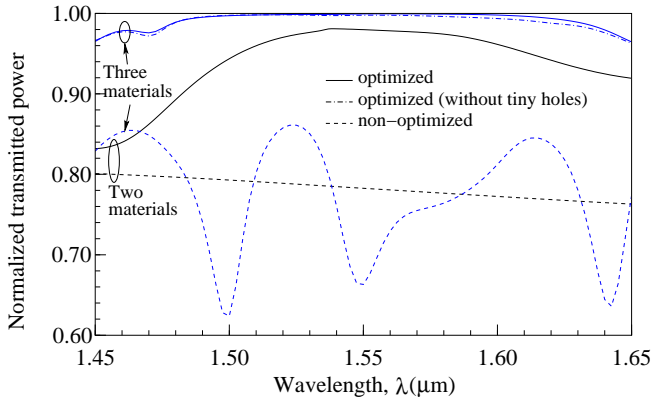
Fig. 9. Wavelength dependence of the normalized transmitted power of the non-optimized and optimized structures in the multi-wavelength optimization.
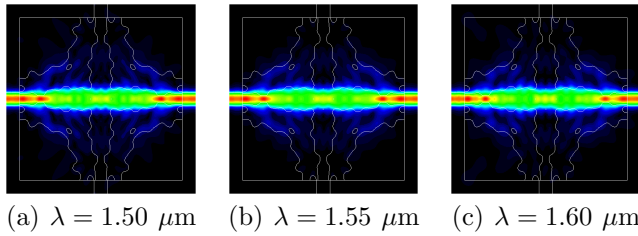


(a) $\lambda = 1.50\ \mu$m  (b) $\lambda = 1.55\ \mu$m  (c) $\lambda = 1.60\ \mu$m

Fig. 10. Propagating field in waveguide crossing with three materials.



(a) $\lambda = 1.50\ \mu$m  (b) $\lambda = 1.55\ \mu$m  (c) $\lambda = 1.60\ \mu$m
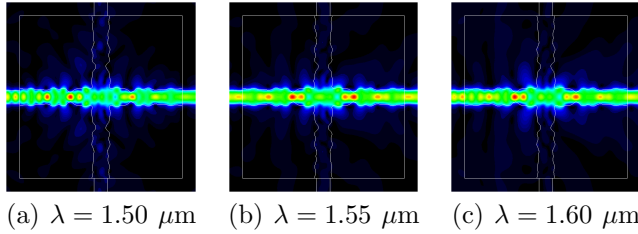
Fig. 11. Propagating field in waveguide crossing with two materials.



with gray area    without gray area
(a) two materials



with gray area    without gray area
(b) three materials



(c) wavelength dependence

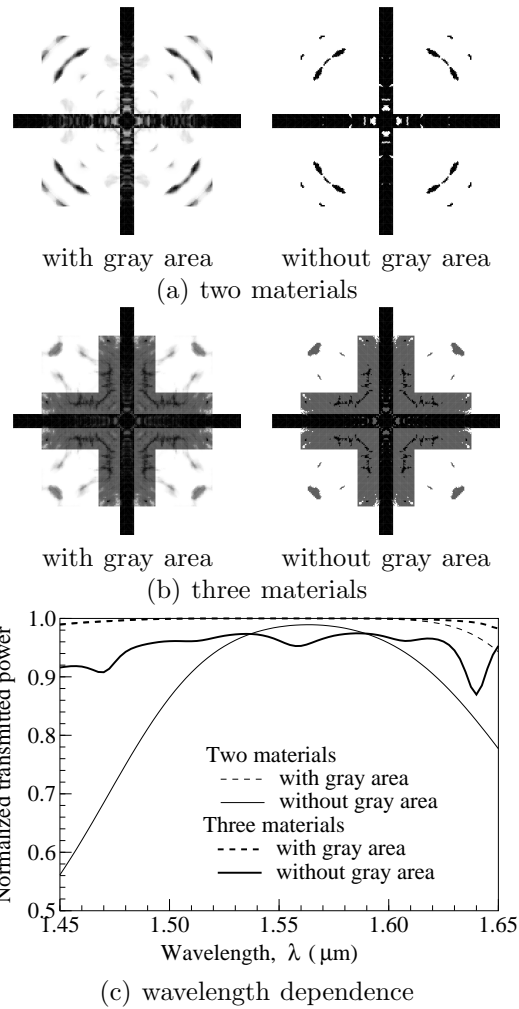Fig. 12. Results of topology optimization based on the density method. (a) and (b) Optimized structures. (c) Wavelength dependence of the normalized transmitted power of the optimized structures.

crossing with two materials shows stronger wavelength dependence because of its higher refractive index difference than that of the optimized waveguide crossing with three materials, in which refractive indices of its core and first cladding are, respectively, $n_1 = 2.73$ and $n_2 = 2.1$. Since it is hard to process four tiny holes in the optimized structure of Fig.6(d), we also show in Fig. 9 the result for the optimized structure with the tiny holes filled with the material of $n_2 = 2.1$. We find that it is almost the same as that for the optimized structure of Fig. 6(d).

The propagating fields in the optimized structure are shown in Figs. 10 and 11. In the structure obtained with two materials, the relatively large radiated fields are observed because of high refractive index contrast. On the other hand, in the structure obtained with three materials, we can see that the radiated fields are suppressed by two material boundaries and the light is concentrated by lens-like effect around crossing region.

Finally, in order to compare waveguide crossings in the function expansion method and the density method, we

show the optimized structure based on the density method with two materials in Fig. 12(a) and that with three materials in Fig. 12(b). Since the optimized structure in the density method has gray areas, we also show the optimized structure without gray area in those figures. Fig. 12(c) shows the wavelength dependence of the transmitted power of the optimized structures with/without gray area. The transmitted power of the optimized structure with gray area is almost unity over the wavelength of 1.5 to 1.6 $\mu$m, but the optimized structure without gray area in the density method has many tiny structures which it may be hard to process, and its transmitted power is lower than that shown in Fig. 9 for the optimized structure in the function expansion method.

## IV. Conclusion

In this study, we proposed the optimization using the multi-materials in the topology optimization based on the function expansion method. We actually demonstrated the optimization examples for waveguide crossing and confirmed its effectiveness.

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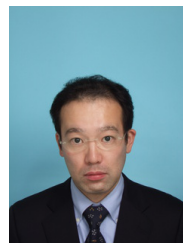
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