A Study on Topology Optimization of Plasmonic Waveguide Devices Using Function Expansion Method and Evolutionary Approach

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A Study on Topology Optimization of Plasmonic Waveguide Devices Using Function Expansion Method and Evolutionary Approach

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Abstract—We propose a novel topology optimization method for plasmonic devices. Plasmonic devices which have a great potential to downsize various optical devices beyond the diffraction limit attract a lot of attention. In order to develop high-performance plasmonic devices, a novel design theory is expected to be established instead of the conventional theory for dielectric waveguide devices. In this paper, we employ the function-expansion method to express a device structure in the design region and optimize the design variables by using several evolutionary approaches which do not require the sensitivity analysis. The validity and usefulness of this approach are demonstrated through the design examples of optical diode and optical circulator.

Index Terms—Plasmonic waveguide device, function-expansion method, finite element method (FEM), evolutionary method.

I. INTRODUCTION

In recent years, since the communications traffic is increasing explosively, miniaturization of optical devices and capacity enlargement of optical communication systems are more and more required. Most of the conventional optical waveguide devices are developed by using dielectric waveguide materials and those waveguide devices have a limitation for downsizing because of the diffraction limits. On the other hand, plasmonic waveguide devices have a possibility to be miniaturized beyond the diffraction limit by utilizing the large negative refractive index of metal. Therefore, plasmonic devices attract a lot of attention and are intensively studied in recent years to develop ultra-compact photonic devices [1]–[4]. Under these circumstances, in order to develop high-performance plasmonic devices beyond the conventional design theory, a novel design approach is expected to be developed.

Topology optimization method which has been developed to design optical devices in recent years has high flexibility and has a possibility to discover unique device structures without requiring designer’s experiences. Several dielectric waveguide devices have been designed so far [5]–[8]. However, the topology optimal design for plasmonic devices seems to have not been well discussed. Although gradient based topology optimization based on the sensitivity analysis by the adjoint variable method can efficiently find out an innovative device structure, the obtained structure sometimes depends on an initial structure and moreover the sensitivity of plasmonic devices to the structural deviation is relatively high and is sometimes localized because of a large negative refractive index of metal. As a result, the structural update is localized and it is sometimes difficult to find out an innovative device structure independent of an initial structure. Especially when the conventional density method [6] is used for the representation in the design region, fine structures sometimes emerge and the light intensity and the sensitivity tend to be localized. On the other hand, when using the function-expansion based refractive index representation, device structure can be expressed with a small number of design parameters and the smooth material boundary can be easily obtained [7]. However, in the previous discussion of the function-expansion based topology optimization is limited to dielectric devices and the material boundary is not rigorously treated because of the existence of the narrow gray area.

In this study, for the purpose of making the function-expansion based optimization method applicable to plasmonic waveguide devices, we propose an evolutionarily-based topology optimal design method. In our approach, a device structure in the design region is expressed by using the function-expansion method with a relatively small number of design variables and those design variables are optimized by utilizing several evolutionary approaches. Since the optimized device structure sometimes depends on the basis function of the function expansion method [8], we compare two types of basis function with different characteristics. It is reported that Fourier series is easy to change overall structure and pyramid function is easy to modify the local structure. In addition, finite element mesh generation is improved to make the element boundary fit the material boundaries. Furthermore, in order to optimize design variables, we compare five types of evolutionary approaches: the genetic algorithm (GA), particle swarm optimization (PSO), differential evolution (DE), firefly algorithm (FA) and hybrid FA with DE (HFA) as evolutionary methods. Through the design examples of a plasmonic optical diode and optical circulator, the validity and usefulness of the proposed method are demonstrated.

This paper is organized as follows. In section II, we briefly review the function-expansion method and also explain the adaptive mesh generation. In addition, five evolutionary methods used in this study are briefly described. In section III, We
II. TOPOLOGY OPTIMIZATION

A. Representation of Refractive Index Distribution in Design Region

We consider a plasmonic device whose cladding is metal and core is air as shown in Fig. 1. In ordinary topology optimization, a relative permittivity distribution in the design region is expressed by some numerical design variables and the structure with the desired property is obtained by optimizing these values. In this paper, we employ the function-expansion method to express the relative permittivity in the design region because this method can define clear material boundaries. Here, the relative permittivity in the design region is expressed by the following equation:

\[ \varepsilon_r(y, z) = \varepsilon_{ra} + (\varepsilon_{rb} - \varepsilon_{ra})H(w(y, z)) \]  

(1)

where \( \varepsilon_{ra} \) and \( \varepsilon_{rb} \) is the relative permittivity of two considered materials. The Heaviside function, \( H(\xi) \), whose value is 0 or 1 depending on whether \( \xi \) is negative or positive, is used to binarize the relative permittivity. Here, the structure expressing function \( w(y, z) \) is expressed in the form of superposition of arbitrarily defined basis functions, \( f_i(y, z) \), as follows:

\[ \xi = w(y, z) = \sum_{i=1}^{N} c_i f_i(y, z). \]  

(2)

In this paper, we employ the following two expressions and compare the results obtained by those expressions.

1) Fourier series: The function \( w(y, z) \) can be expressed as follows:

\[ w(y, z) = \sum_{i=-N_x}^{N_x-1} \sum_{j=-N_z}^{N_z-1} (a_{ij} \cos \theta_{ij} + b_{ij} \sin \theta_{ij}) \]  

(3)

\[ \theta_{ij} = \frac{2\pi i}{L_y} y + \frac{2\pi j}{L_z} z \]

where \( N_x \) and \( 2N_z \) are the numbers of expansion terms along \( y \)- and \( z \)-direction, respectively. \( L_y \) and \( L_z \) is the period of Fourier series along \( y \)- and \( z \)-direction, respectively, and those values are set to be greater than the width of the design region along each direction to avoid generating a periodic structure. Fourier series has the potential to efficiently obtain a simpler structure because the device structure can be expressed using a relatively small number of expansion terms.

2) Superposition of pyramid functions: The function \( w(y, z) \) can be also expressed by using pyramid function as follows:

\[ w(y, z) = \sum_{i=0}^{N_x} \sum_{j=0}^{N_z} c_{ij} f(y - y_i, \Delta y, z - z_j, \Delta z) \]  

\[ f(\xi) = \begin{cases} 1 & (|\xi| \leq 1) \\ 0 & (|\xi| > 1) \end{cases} \]  

(4)

where \( (y_i, z_j) \) is the coordinate of the sampling point, and \( \Delta y \) and \( \Delta z \) are the sampling intervals in the \( y \)- and \( z \)-directions, respectively. Since the pyramid function is a locally defined function, it may be superior for local search rather than dramatically changing the topology of device structure when a gradient-based method is used. It is also noted that we have to increase the number of sampling points to get a smooth material boundary. This may degrade the convergence speed in an evolutionary-type optimization.

B. Formulation by the Finite Element Method

In order to evaluate device performances, we employ the finite element method (FEM) because of its versatility, especially its ability to rigorously treat material boundaries. In the case of two-dimensional plasmonic waveguides, the equation which describe light propagating behavior can be written as

\[ \frac{\partial}{\partial y} \left( \rho \frac{\partial \Phi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \rho \frac{\partial \Phi}{\partial z} \right) + k_0 q \Phi = 0 \]  

(5)

with

\[ \begin{cases} p = 1, & q = n^2, & \Phi = E_x \text{ for TE mode} \\ p = 1/n^2, & q = 1, & \Phi = H_z \text{ for TM mode} \end{cases} \]

where \( k_0 \) is free space wave number and \( n \) is a refractive index distribution. Dividing the computational domain into a number of second order triangular elements, and applying the FEM to (5), we can finally obtain a simultaneous linear equation in matrix form as follows [9]:

\[ [P] [\phi] = \{u_{in}\} \]  

(6)

\[ [P] = [K] - k_0^2 [M] \]  

(7)

\[ [K] = \sum_e \int_{\Gamma_e} q(N^T) \frac{\partial(N)}{\partial y} \frac{\partial(N)}{\partial y} + \frac{\partial(N)}{\partial z} \frac{\partial(N)}{\partial z} ddydz \]  

(8)

\[ [M] = \sum_e \int_{\Gamma_e} q(N^T) (N^T) ddydz \]  

(9)

\[ [Q] = -j2\beta_{in} \sum_{\Gamma} \int_{\Gamma} q(N^T) (N^T) ddy \]  

(10)

\[ \{u_{in}\} = [Q] \{\Phi_{in}\} \]  

(11)

where \( \{\Phi\} \) is a vector consisting of the value of \( \Phi \) at all nodes and \( \{N\} \) is the shape function vector. \( \sum_e \) denotes the sum of all elements, \( \sum_{\Gamma} \) denotes the sum of all elements related to incident plane \( \Gamma \), and \( \{u_{in}\} \) is the vector related to the
incidence field.

In the previous study of the function expansion based topology optimization of dielectric waveguides [7], [8], finite element mesh is generated before the optimization and it is not updated during the optimization process. In this case, material boundaries are not rigorously treated and gray areas exist around the material boundary to calculate the sensitivities. Although this is not a significant issue in the case of dielectric devices, it may cause a significant computational error in the case of plasmonic devices because of a high refractive index difference between metal and dielectric. In this study, the gray area is completely suppressed and the material boundaries are rigorously treated by generating finite element mesh fitting to the material boundaries. Figure 2 shows the image comparing the conventional and present meshes. In this paper, first, an almost regular mesh with a sufficient number of elements is prepared and the elements which include material boundary is subdivided into three elements. That is, a triangular element is subdivided into a triangle and a rectangle at the material boundary and the rectangle is subdivided into two triangles. The adaptive refinement of finite element mesh or the improvement is able to be followed if necessary [10], [11]. In this technique, if the number of design variables \((N_p \times N_z)\) is large, the initially prepared mesh should be sufficiently fine to avoid a complicated curve in a finite element. However, in general, the number of design variables should be sufficient small compared with the number of finite elements to avoid unrealistic complex structure.

C. Evolutionary Method to Optimize Design Variables

In our previous topology optimization method of dielectric devices based on the function expansion method, we employ a gradient method based on the adjoint variable method to optimize design variables. However, in plasmonic devices, we sometimes face the problem that light localizes around fine structures, as a result, the sensitivity also localizes around there, and an update of the device structure is also often localized. Hence, we employ evolutionary approaches to optimize design variables. These methods have a possibility to find the global optimal solution by searching with a number of diverse solutions in a solution space. In this paper, we employ the following five algorithms.

1) Genetic Algorithm (GA): GA is the algorithm based on natural selection [12] and widely used to solve various design problems because of its extensive applicability. In GA, an initial population is randomly generated and some individuals in it are selected according to their fitness values to succeed their genetic information to the next generation. New children, \(x_{c}^{(n+1)}\), in the next generation are generated by a crossover of the two selected parents, \(x_{p1}^{(n)}\) and \(x_{p2}^{(n)}\), as follows:

\[
x_{c}^{(n+1)} = w x_{p1}^{(n)} + (1-w)x_{p2}^{(n)}
\]

where \(w\) means the random number \((w \in [0, 1])\). In addition, GA randomly mutates the genetic information of individuals by a given probability to avoid falling into a local solution.

2) Particle Swarm Optimization (PSO): PSO is the algorithm that imitates the social behavior of organisms like birds and fishes [13]. This algorithm searches the solution space based on the information shared among a swarm of particles. The current position \(x_{i}^{(n)}\) and velocity \(v_{i}^{(n)}\) of \(i\)-th particle are updated using the following equations:

\[
x_{i}^{(n+1)} = x_{i}^{(n)} + v_{i}^{(n+1)}
\]

\[
v_{i}^{(n+1)} = w v_{i}^{(n)} + r_{1}C_{1}(x_{p}^{(n)} - x_{i}^{(n)}) + r_{2}C_{2}(x_{g}^{(n)} - x_{i}^{(n)})
\]

where \(x_{p}^{(n)}\) and \(x_{g}^{(n)}\) are the best positions which have found by the \(i\)-th particle and all the particles, respectively, until \(n\)-th iteration. \(w\) is an inertial coefficient, \(C_{1}\) and \(C_{2}\) are the coefficients which are related to the force from \(x_{p}^{(n)}\) and \(x_{p}^{(n)}\). \(r_{1}\) and \(r_{2}\) are randomly selected numbers \((r_{1}, r_{2} \in [0, 1])\).

3) Differential Evolution (DE): In DE algorithm, a mutant individual is generated using the differential vector between arbitrarily selected individuals and a new individual is generated by the crossover between the current and mutant ones [14]. A mutant individual \(x_{m}^{(n)}\) is generated as follows:

\[
x_{m}^{(n)} = x_{p1}^{(n)} + F(x_{p2}^{(n)} - x_{p3}^{(n)})
\]

where \(x_{p1}^{(n)}, x_{p2}^{(n)}\) and \(x_{p3}^{(n)}\) are randomly selected individuals, \(F\) is a scale factor \((F \in [0, 1])\). Since the differential vector, \(x_{p2}^{(n)} - x_{p3}^{(n)}\), becomes small through an iteration process, the search in DE transitions from global search to local search.

4) Firefly Algorithm (FA): FA is an algorithm developed inspired by the courtship behavior of fireflies [15]. In FA, current individuals are attracted by all more attractive individuals according to the attractiveness and distance. The position of the current individual, \(x_{i}^{(n)}\) is updated as the following equation:

\[
x_{i}^{(n+1)} = x_{i}^{(n)} + \sum_{j}u(\beta_{0,j} - \beta_{0,i})\beta_{0,j}e^{-\gamma r_{ij}^{2}}(x_{j}^{(n)} - x_{i}^{(n)})
\]

\[+ \alpha \delta^{n} \varepsilon\]

where \(u(\xi)\) is the unit step function, \(\beta_{0,j}\) is the attractiveness of \(j\)-th individual, \(r_{ij}\) is the distance between \(x_{i}^{(n)}\) and \(x_{j}^{(n)}\), and \(\gamma = 1/\sqrt{L}\) is the light absorption coefficient. Here, \(L\) is a quantity which decides a search range of each individual. \(\alpha\) is a scale factor, \(\delta\) is a damping coefficient, and \(\varepsilon\) is a random vector where each component lies in \([-1, 1]\).

5) Hybrid Firefly Algorithm (HFA): HFA is the hybrid method of DE and FA [16]. In HFA algorithm, the initial population is divided into two groups with its half size and each group evolves using DE or FA, then new individuals in both groups are mixed and regrouped. HFA algorithm has a potential to obtain a global optimum by utilizing the advantages of both algorithms.
III. OPTIMAL DESIGN EXAMPLES OF PLASMONIC WAVEGUIDE DEVICES

A. Plasmonic Optical Diode

We consider an optical diode in which the light transmits in the forward direction and the backward transmission is prohibited [17]. The design model of a plasmonic diode is shown in Fig. 3 and the fundamental TM mode operation is considered. The operation wavelength is assumed to be $\lambda = 1.55 \mu m$. In this paper, the permittivity of metal is expressed by using the Lorentz-Drude model [18], the permittivity of silver is calculated as $\varepsilon_{Ag} = -103.33 - j8.1302$ when $\lambda = 1.55 \mu m$. The relative permittivity of air is assumed to be $\varepsilon_{air} = 1$. The waveguide width is $w = 0.8 \mu m$, the PML thickness is $d = 0.5 \mu m$, and the design region width in the $y$- and $z$- directions are $W_y = 0.8 \mu m$ and $W_z = 1.5 \mu m$, respectively. In order to realize diode operation by using only reciprocal materials, the fundamental mode from port 1 should be converted to the higher order mode in port 2 and the transmission of the fundamental mode from port 2 to port 1 should be prohibited. Thus, the objective function to be minimized is given as follows:

$$
C = (0 - |S_{21}^{(0)}|^2)^2 + (1 - |S_{21}^{(1)}|^2)^2
+ (0 - |S_{12}^{(0)}|^2)^2 + (0 - |S_{12}^{(1)}|^2)^2
$$

(17)

where the superscripts of $S$-parameters denote mode number of the transmitted mode.

The number of iteration steps is set to be 1000. The number of population $N_p$ is set to be 32, 64, or 128. Here, the parameters used in each evolutionary approach are set as follows: the mutation rate is 0.01 in GA, $w = 0.9$ in PSO, $F = 0.5$ in DE, and $\alpha = 0.1$, $\beta = 2.0$ and $\delta = 0.999$ in FA, respectively. These parameters were determined through preliminary optimizations for the following design problem of a plasmonic diode while varying the values of these parameters. However, the optimum values of these parameters may depend on a design problem and we cannot decide which optimization method is superior to the others at the present stage. Therefore, we think that to use some different optimization approach is effective for us to get higher-performance plasmonic devices.

In this example, as a structure expressing function, $w(y, z)$, we consider the pyramid function and Fourier series.

1) Pyramid function: We consider the pyramid function as a structure expressing function, $w(y, z)$. The number of expansion function along the $y$- and $z$- directions are set to $N_y = 16$ and $N_z = 32$, respectively. Figure 4 shows the objective function as a function of the iteration step. We can see that the value of the objective function is improved in the iteration process. The transmittance of the optimized structure obtained by each evolutionary approach is summarized in Table I. In these optimizations, the best performance is obtained in the optimized structure by HFA with $N_p = 128$. In this device, the forward transmittance of $|S_{21}^{(1)}|^2 = 0.84$ is obtained and the backward transmittance is suppressed to $|S_{12}|^2 = |S_{12}^{(0)}|^2 + |S_{12}^{(1)}|^2 = 0.010 \times 10^{-3}$. Figure 5 shows the propagating fields in the three optimized plasmonic diodes with better performance. We can see that the optimized structure is complicated because the pyramid function requires a lot of design variables, $N_y \times N_z$, to express a smooth structure avoiding staircase geometry.

2) Fourier series: We consider Fourier series as $w(y, z)$.

The number of expansion functions along the $y$- and $z$-directions are set to $N_y = 2$ and $N_z = 8$, respectively, and the Fourier periods, $L_y$ and $L_z$, are set to be $L_y = 1.2 W_y$ and $L_z = 1.2 W_z$, respectively. Figure 6 shows the objective function as a function of the iteration step. We can also see that the value of the objective function is improved in the iteration process. The transmittance in the optimized structure obtained by each evolutionary approach is summarized in Table II. In these optimizations, the best performance is obtained in the optimized structure by HFA with $N_p = 128$. In this device, the forward transmittance of $0.85$ is obtained and the backward transmittance is suppressed to $0.20 \times 10^{-3}$. The propagating fields in the three plasmonic diodes with better performance are shown in Fig. 7. In the forward propagation, we can observe that the fundamental TM mode is converted into the first higher mode in port 2 and the discontinuous structure around the entrance of port 2 reflects the fundamental TM mode from port 2 in backward propagation. From these results, we can see that the optimized structure is simpler than that by
B. Plasmonic Optical Circulator

Next, we consider an optical circulator in which the light incident in any port transmits to the next port in a counter-clockwise rotation [2]. Figure 9 shows the design model of a plasmonic circulator. The wavelength is assumed to be $\lambda = 1.55$ $\mu$m and the fundamental TM mode operation is considered. The structural parameters are assumed to be $d_{\text{bus}} = 0.8$ $\mu$m, $L_1 = 2.2$ $\mu$m, $L_{\text{bus}} = 2.35$ $\mu$m, and $W_y = W_z = 3$ $\mu$m. Considering the desired device operation, the optimized structure should have 90-degree rotational symmetry. Thus, we impose a 90-degree rotational symmetry condition and use the following objective function to be minimized:

$$\text{Minimize } C = (0 - |S_{21}^{(0)}|^2 + (1 - |S_{21}^{(1)}|^2)^2. \quad (18)$$

In order to prevent the transmission of the fundamental mode from port 2 to port 1, the fundamental mode transmission is suppressed and the higher order mode transmission is maximized. Although only the port 1 incidence case is considered, the other ports incidence cases are automatically satisfied due to the rotational symmetry condition. We consider only Fourier series as a structure expressing function, $w(y, z)$, to obtain a simpler optimized structure. The number of expansion function along the $y$- and $z$- directions are set to be $N_y = N_z = 8$ and the Fourier periods are set to be $L_y = 1.2W_y$ and $L_z = 1.2W_z$, respectively. The settings of the evolutionary approaches are the same in the previous design example.
Figure 8. Wavelength dependence of the normalized transmitted and reflected power in the optimized plasmonic optical diode which is obtained by HFA with $N_\mu = 128$ when Fourier series is employed as $w(y, z)$.

Figure 9. Design problem of a plasmonic optical circulator surrounded by PML.

Figure 10 shows the objective function as a function of the iteration step. These results show the objective function rapidly decreases at the initial stage of the optimization process. In addition, in this design example, we can see that the good performance is obtained by HFA and DE even with less number of population. The transmittance in the optimized structure obtained by each evolutionary approach is summarized in Table III. In these optimizations, the best performance is obtained in the optimized structure by HFA with $N_\mu = 32$ and the transmission to the desired port of 0.83 and the crosstalk rejection of $2.89 \times 10^{-3}$ in the worst port are achieved. The propagating fields in the three plasmonic circulators with better performance are shown in Fig. 11. We can see that the almost same structures are obtained in these optimizations. Figure 12 shows the wavelength dependence of the normalized transmission power into port 2 and the crosstalk to the other ports, in the optimized device by HFA with $N_\mu = 32$. The crosstalk to port 3 is well suppressed although this is not explicitly considered in the objective function. This is because this rejection is implicitly considered by suppressing $|S_{21}(0)|^2$, due to the symmetrical and reciprocal operation. On the other hand, the reflectance has slightly stronger wavelength dependence compared to the crosstalk.

In these optimizations, the optimized device structure may be complicated in some cases. The use of Fourier series as a structure expressing function has a possibility to suppress such complicated fine structures, compared with the use of pyramid functions. In order to get further simplified the optimized structure, it is shown that the application of the structural smoothing filter is effective [19]. In the case of using Fourier series, components of higher frequency can be efficiently

![Graph showing wavelength dependence of normalized power](image)

![Diagram showing design problem](image)

![Table III](image)

![Optimized structures](image)

![Graph showing objective function](image)
suppressed by using Gaussian Filter.

Although only two materials are considered in these design examples, three or more materials can be also treated by using the function expansion method [20]. We think three-dimensional structure is also able to be optimized in the same optimization framework because the function-expansion based topology optimization for three-dimensional waveguide has been already discussed [21]. However, it requires far longer computational time compared with two-dimensional problems and more efficient optimization approach is expected to be developed. Utilizing the gradient-based topology optimization [21] in the present evolutionary approach may accelerate the convergence and that is our future work.

IV. CONCLUSION

We proposed the novel topology optimization method of plasmonic waveguide devices. As design examples, a plasmonic optical diode and circulator are designed by using our proposed method. From these results, it is shown that, as the structure expressing function, Fourier series has an ability to express smooth and simple device structure with fewer design parameters compared to the pyramid function. We tested the five evolutionary methods and we are now thinking that the better approach depends on a design example. In the future, we will study the hybrid optimization method that combines an evolutionary approach which has an ability to search a global optimum with a gradient-based approach which has an ability of efficient local search.

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