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NANO-APERTURE DESIGN FOR VERTICAL-CAVITY SURFACE-EMITTING LASER USING THE SHAPE OPTIMIZATION PROCEDURE

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1. Abstract
This study suggests a systematic design approach of a nano-aperture for the purpose of improving optical transmission enhancement. The vertical-cavity surface-emitting laser (VCSEL) is one of the prospective applications of the nano-aperture and it is widely used in the optical communication or near field memory for high-density recording. In the design process, we adopt the phase field method based shape optimization procedure using a reaction-diffusion equation which is a kind of shape optimization method. We solve the optimization problem using five different initial configurations, which greatly affect the optimization results. The finite element method (FEM) is implemented by the commercial package COMSOL ver. 3.5a, and the optimization process is carried out by Matlab programing.

2. Keywords: Vertical-cavity surface-emitting laser, Phase field method, Finite element analysis

3. Introduction
The VCSEL is widely used in many fields such as optical memory, optical printers and optical signal transmission. To enhance efficiency of a VCSEL, it is essential to obtain the optimal of cross section of the nano-aperture in the VCSEL. In optics, challenging Bethe's prediction about diffraction limit [1], many researchers proposed various structures whose transmission efficiency of the nano-aperture is larger than 1. Appropriate sub-wavelength nano-aperture shape in the metallic layer such as C-shaped [2] or bowtie apertures [3] can overcome the prediction about the diffraction limit. The grating structure of the metallic layer is also studied and proposed for higher performance in the optical near field [4]. However, most of them studied pre-existing ridge-type shapes and used applications of the parameter optimization approach limited in old shaped models [5].

Since the earliest concept of topology optimization proposed by Bendsøe and Kikuchi [6], topology optimization is regarded as one of the most effective tools for structural design. In contrast with traditional methods like size or shape optimization, topology optimization can make radical design evolution beyond initially proposed models. One of the famous topology optimization methods, the solid isotropic material with penalization (SIMP) method is considered as an easy approach of optimization. In the SIMP method, a material property distribution is determined in accordance with the element density value [7]. It has been widely used in compliant mechanism design [8], structural design in magnetic fields [9] and design in electromagnetic wave problems [10].

Another widely used topology optimization method is so called the level set method based on the implicit interface [11-13]. It is a numerical technique for boundary tracking and uses the iso-surface scalar level set function updated by the Hamilton-Jacobi formulation. The result by the level set method clearly shows smooth boundaries and it is used in many physical fields like SIMP method [11-15].

Recently, for need to cover disadvantage of above optimization methods, the phase field method was proposed [16]. The optimization scheme is a tracking method that tracks material boundaries related with the objective value and it does not require the re-initialization procedure. The phase field method is modified by Takezawa et al. [17] and Choi et al. [18]. They used reaction-diffusion (RD) equation to update design variables and control the diffusivity by controlling the diffusion term in RD equation. Recently, Choi et al. [19] combined two methods mentioned above and applied to the magnetic field problem.

In this study, we have expanded the application range of phase field topology optimization into electromagnetic wave field problems and designed the optimal cross sectional shape of the metal layer in a VCSEL system. The design domain composed of metal and dielectric material is associated with the wave propagation analysis using the surface plasmon (SP) effect. Furthermore, unlike former topology optimization of electromagnetic fields, the design domain of structure is located in the output surface of incident beam in the optimization process. This study adopts the RD equation and double well potential (DWP) combined topology optimization method not only for removing gray scale but also for obtaining simple structure shape.

4. Analysis of two dimensional (2D) nano-aperture

In this section, we explained the 2D nano-aperture analysis. We use the FEM to analyze nano-aperture system. The electromagnetic wave propagation can be analyzed by solving the Maxwell's equations and the Maxwell's equations for time-varying fields are as follows:

$$\nabla \times \nabla \times \mathbf{E} = -\mu\varepsilon \frac{\partial^2}{\partial t^2}\mathbf{E} \tag{1}$$

$$\nabla \times \nabla \times \mathbf{H} = -\mu\varepsilon \frac{\partial^2}{\partial t^2}\mathbf{H} \tag{2}$$

where **E** is the electric field vector and **H** is the magnetic field strength. ε and μ represent the electric permittivity and the magnetic permeability, respectively. In Eq. (2), the transverse magnetic (TM) mode equation is the governing equation of the system, so it can be rewritten without their dependency on time and in the use of speed of light c and wave frequency of ω.

$$\nabla \cdot \left(\frac{1}{\varepsilon_r} \nabla \mathbf{H} \right) = -\left(\frac{\omega}{c_0} \right)^2 \mathbf{H} \tag{3}$$

where $c_0 = 1/\sqrt{\mu_0 \varepsilon_0}$ is the speed of light in the vacuum or air, ε_r is the relative permittivity, ε_0 is the permittivity in vacuum or air, μ_0 is the magnetic permeability in vacuum or air. In the 2D system, when we only used H_z for TM mode, the governing equation of a propagation wave in a nano-aperture system is written as follows.

$$\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon_r}\frac{\partial}{\partial x} H_z \right) + \frac{\partial}{\partial y}\left(\frac{1}{\varepsilon_r}\frac{\partial}{\partial y} H_z \right) = \frac{\omega^2}{c_0{}^2} H_z \tag{4}$$

The design objective is to maximize the Poynting vector in the measuring area and it can be represented as follows in harmonic cases:

$$\langle \mathbf{P} \rangle = \frac{1}{2}\Re\left(\mathbf{E} \times \overline{\mathbf{H}} \right) \tag{5}$$

where < > means a time averaged value, $\overline{\mathbf{H}}$ means the complex conjugated value of the magnetic field strength vector and $\Re(\ )$ means the real value of ( ).

5. Design methods

Our approach uses the RD equation for updating design variables. The equation is composed of two different processes, namely as the reaction term and the diffusion term. We use DWP function in the reaction term, and thereby this approach enables the boundary tracking.

5.1 Optimization algorithm

The RD equation used for topology optimization in this study is formulated as

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = \alpha \nabla^2 \phi(\mathbf{x},t) - \frac{\partial P(\phi, H_z)}{\partial \phi} \qquad in \quad \mathbf{x} \in \Omega, \quad 0 < t \le T \tag{6}$$

$$\frac{\partial \phi}{\partial \mathbf{n}} = 0 \qquad on \quad \partial\Omega \tag{7}$$

where $\Omega \subset \mathbf{R}^N$ is a bounded domain with boundary $\partial\Omega$, ϕ is the design variable which represents a phase field parameter. T represents the time required for the density field convergence and **n** is the unit vector normal to $\partial\Omega$. α means the diffusion coefficient.

For optimization for minimize the Poynting vector in systems considering the equality volume constraint, the optimization problem is written as follows:

$$\underset{\phi}{\textbf{minimize}} \quad P(\phi,\, H_z)$$
$$\textbf{subject to} \quad h(\phi) = \int_\Omega \phi\, dx - V_{req} \int_\Omega dx \le 0,\ 0 \le \phi \le 1 \tag{8}$$

where P is the objective function, $h(\phi)$ means the volume fraction constraint and V_{req} is the required volume fraction. To deal with the design constraints, the augmented Lagrangian is defined as

$$\overline{P}(\phi, H_z, \lambda) = \eta P(\phi, H_z) + \lambda \hat{h}(\phi) + \frac{\gamma}{2} \hat{h}(\phi)^2 \tag{9}$$

Here, λ represent the Lagrange multiplier, γ is the penalty parameter and η is value to normalize the sensitivity. The gradient of the Lagrangian with respect to the density field is employed as the reaction term in (6).

$$\frac{\partial \overline{P}(\phi, H_z, \lambda)}{\partial \phi} = \eta \frac{\partial P(\phi, H_z)}{\partial \phi} + \frac{\partial \hat{h}(\phi)}{\partial \phi} \left[\lambda + \gamma \hat{h}(\phi) \right] \tag{10}$$

For topology optimization using the DWP function, the gradient of augmented Lagrangian is modified as

$$\frac{\partial \phi}{\partial t} = \alpha \nabla^2 \phi - a w'(\phi) - \left[\eta \left. \frac{\partial P(\phi, H_z)}{\partial \phi} \right|_{t=t_1} + \frac{\partial \hat{h}}{\partial \phi} \left(\lambda + \gamma \hat{h}(\phi) \right) \right] g'(\phi) \tag{11}$$

where $w(\phi) = \phi^2 (1-\phi)^2$, $g(\phi) = \phi^3 (6\phi^2 - 15\phi + 10)$. The function $w(\phi)$ is a smooth Dirac delta function and $g(\phi)$ is a smooth Heaviside function in the range of $0 \le \phi \le 1$. The Heaviside function $g(\phi)$ is applied only to the objective function term to allow the boundary moving along the outer range of the design domain [17, 19].

5.2 Design variables and sensitivity analysis

During the design process, refractive index values in the design domain are changed according to the variation of the design variable, i.e., the phase field parameter ϕ based on the following formulation [20, 21]:

$$n = n(\phi) = n'_{Ag} + \phi^p (n'_{a-Si} - n'_{Ag}) + i(n''_{Ag} + \phi^p (n''_{a-Si} - n''_{Ag})) \tag{12}$$

where n'_{Ag} and n'_{a-Si} are real parts of the refractive index of the silver (Ag) layer and the amorphous silicon (a-Si) part, respectively, and n''_{Ag} and n''_{a-Si} are their imaginary part values.

The derivation of the sensitivities can be performed by the adjoint method [22]. The governing equation of the dynamic problem is defined as

$$\mathbf{KH} = \mathbf{Q} \tag{13}$$

where $\mathbf{K}$ is the stiffness matric, $\mathbf{H}$ is the field vector and $\mathbf{Q}$ is the load vector. Using the chain rule, the sensitivity of the design object P to the design variable ϕ is given by [23]

$$\frac{d\mathrm{P}}{d\phi} = \frac{\partial \mathrm{P}}{\partial \phi} - \lambda^T \left(\frac{\partial \mathbf{K}}{\partial \phi} \mathbf{H} - \frac{\partial \mathbf{Q}}{\partial \phi} \right) \tag{14}$$

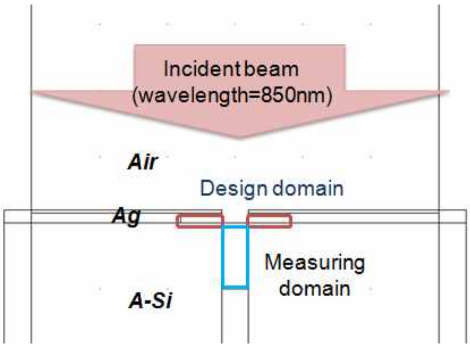
The adjoint variable λ is given as

$$\mathbf{K}^T \lambda = -\frac{\partial \mathrm{P}}{\partial \mathbf{H}} \tag{15}$$

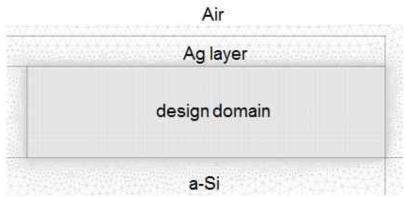
6. Numerical results

6.1 Model description

The initial nano-aperture model is illustrated in Fig. 1(a). In this study, the incident light wavelength is fixed to 850nm, which is in near infrared wavelength range, goes from the upper air portion and passes through the nano-aperture and propagates a-Si layer as displayed in Fig. 1(a). The design domain is defined 75nm depth and 300 nm width silver layer designated in the red box in Fig. 1(a). The design domain is discretized by map-meshing as displayed in Fig. 1(b).



(a)



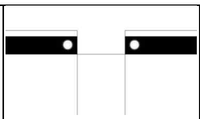
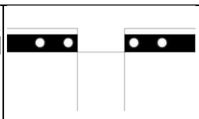
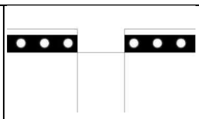
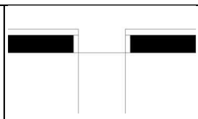
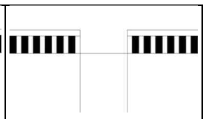
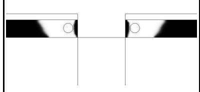
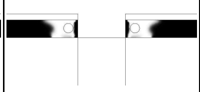
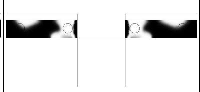
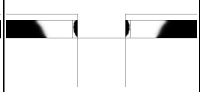
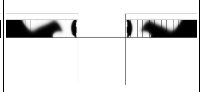
(b)

Figure 1: Initial model of the nano-aperture: (a) schematic for the analysis and (b) element description for FEM

6.2 Influences of the initial configuration

In this section, we consider five initial material distribution for RD equation based design and the optimized results are given in Table 1. The objective is maximizing the Poynting vector and those values are normalized based on the prototype aperture shape. The clear topological shapes are shown in the results and the Poynting vector value is the biggest at the result initiates from the grating structure. Each of optimized configurations differs from the initial material distribution and it is confirmed that the performance of the resultant nano-aperture is seriously influenced by the material distribution near the aperture area.

Table 1: Initial distribution for the phase field method, optimal shape and objective values

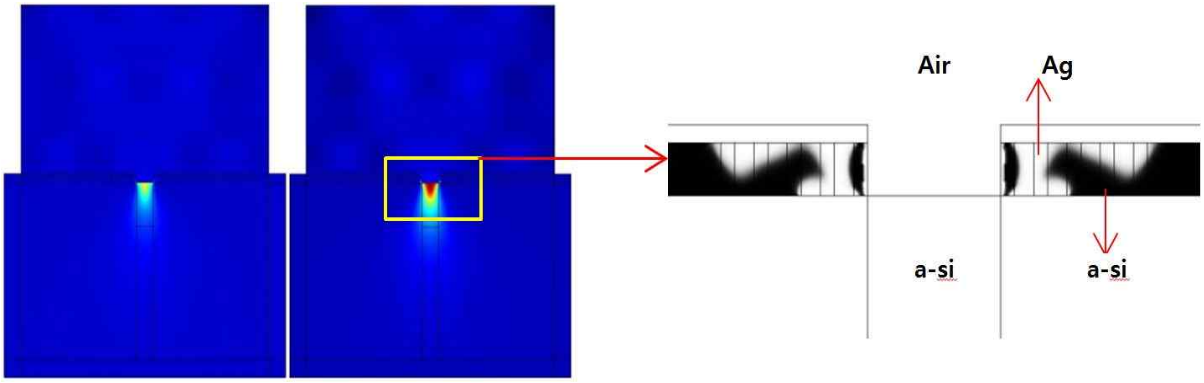
Initial material distribution					
Optimal material distribution					
Normalized objective value	1.75	2.01	1.51	1.73	2.21

6.3 Suggested model

We suggested the optimized nano-aperture shape for a VCSEL system when the volume fraction is set to 0.6. As mentioned before, when we use the RD equation for updating the sensitivity value, we can control complexity of optimized configurations. Therefore, we have attempted changing diffusivity parameter from 1e-3 to 1e-5 and select 1e-4 for in the suggested optimal case. Figure 2(a) shows the Poynting vector contour of the initial model and the optimal model. We could easily confirm the magnitude of the Poynting vector value of the optimal model is much bigger than that of the initial model and over 120% performance improvement of the optimal model can be measured. Figure 2(b) represents the optimal material distribution composed of Ag and a-Si.

7. Conclusions

In this study, the optimal cross sectional shape of the metal layer in a VCSEL is suggested and we confirm the usefulness of the RD equation based design method for electromagnetic wave propagation problems. This approach enables the boundary tracking with DWP functions but does not need the re-initialization process. Although the result with RD equation was dependent on the initial configuration, we have obtained a remarkably improved performance.



(a) (b)

Figure 2: Analysis and material distribution of the suggested optimal model; (a) Poynting vector distribution of initial and optimal model and (b) material distribution of the suggested model

8. Acknowledgment

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