10th World Congress on Structural and Multidisciplinary Optimization
May 19 -24, 2013, Orlando, Florida, USA

TOPOLOGY OPTIMIZATION OF SILVER NANO-PARTICLES IN THIN FILM SOLAR CELLS

Soohwan Byun[1], Jeonghoon Yoo[2]

[1] Graduate School of Mechanical Engineering, Yonsei University, Seoul, Korea, anshar@empas.com
[2] School of Mechanical Engineering, Yonsei University, Korea, Seoul, yoojh@yonsei.ac.kr

Abstract
There are many advantages of using thin film solar cells such as low cost and various applications. However, the drawback interrupting the use of thin film solar cells in practical field is low energy transform efficiency. Therefore, various researches are performed to overcome the problem. One of those researches is using the surface plasmon effect. It is a kind of amplification effect caused by metal-dielectric interactions and generates a strong electric field around metal nano particles [1]. In this study, the surface plasmon effect was used for the efficiency improvement by inserting silver (Ag) nano-particles in the absorbing layer of a thin film solar cell [2-9]. The surface plasmon effect is sensitive to optical properties determined by shape of metal nano-particles [10]. To enhance the effect for improving efficiency, the appropriate shape of metal nano-particles should be determined.

This study adopts the topology optimization method in deciding the shape of metal nano-particles. The update algorithm used in the optimization process is based on the reaction-diffusion equation combined with the double-well potential function [11, 12]. Topology optimization based on the reaction-diffusion equation may be classified as a kind of phase field method which makes phase change occurs only around boundaries. Therefore, the optimal shape of metal nano-particle derived from the phase field method can avoid grey-scale problem and high computational load [12].

In this study, we designed optimal shape of Ag nano-particle by using the level-set method based on the reaction-diffusion equation for improving the efficiency of thin film solar cells. The simulation was performed using the commercial package COMSOL and Matlab. Optical properties used in the simulation and the optimization processes were determined at the specified wavelength of the incident light as 800nm since the thin film solar cell dose not absorb the incident light well, especially at longer wavelengths of sunlight. Finally, the efficiency improvement the thin film solar cell is checked via numerical simulations.

Keywords: Thin film solar cell, Phase-field method, Surface plasmon effect

1. Introduction

The low efficiency problem of thin film solar cells restricts a variety of its applications for practical use. The surface plasmon effect stems from the metal-dielectric interaction could be a solution of low efficiency problem [2-9]. The principle of surface plasmon for improving low efficiency is that insertion of metal nano particles and structures can amplify electric field around the absorbing layer composed of dielectric material [1]. Enhanced electric fields make thin film solar cells absorb more light in the absorbing layer. There are many applications improving electric fields in the dielectric absorbing layer using the surface plasmon effect. Design of nucleated nano-particles for inducing the surface plasmon effect was proposed by Chen et al [13]. Zhu et al. [14] proposed a nano-shell composed of multi-phased material and Liu et al. [15] checked surface plasmon effect using metal nano-particles through experiments. Furthermore, Mertens et al. [16] proposed Ag nano-particles array in the silicon layer for using the surface plasmon effect. In this study, we designed shape and size of Ag nano-particles in the unit-structure of a thin film solar cell to improve the surface plasmon effect for the purpose of increasing the efficiency of the thin film solar cell.

The surface plamson effect can be generated by inserting metal nano-particles in the absorbing layer. However, the shape and size of metal nano-particle must be carefully determined to improve and maximize the surface plasmon effect. The reason of the importance of the metal nano-particle shape and size is that the surface plasmon effect is sensitive to optical properties of metal nano-particles determined by shapes of nano-particles [10]. In this study, we used the level set optimization scheme based on the reaction-diffusion equation to get the optimal shape and size of metal nano-particles.

Topology optimization is regarded as a useful optimization method for deciding the optimal material distribution. However, two representative methods of topology optimization, the solid isotropic material with penalization (SIMP) method and the homogenization design method (HDM), have drawbacks such as intermediate density of elements, heavy computational work and checkerboard pattern [17-19]. The level-set method was

proposed to resolve those drawbacks [20-21]. The difference between the level-set method and traditional topology methods is that the design variable of level-set method is defined along the material boundary. The design variable setting makes the material phase change generate only around the boundary. Therefore, optimal design of a structure can avoid intermediate density distribution and heavy computational work. There are many methods of level-set method. Among them, this study adopts the level-set method based on reaction-diffusion equation, which is a modified method of a phase field method [22] to find optimal design of nano-particles in the absorbing layer of thin film solar cells.

The reaction-diffusion equation is the equation combined with the reaction term and the diffusion term. Reaction means interaction between two substances composing system and the diffusion term represents distribution of two substances. Since the reaction-diffusion equation is suitable for representing phase change, the reaction-diffusion equation is used as an update algorithm in the topology optimization process. However, contrary to traditional level-set methods, topology optimization using the reaction-diffusion equation is different from the classical level-set method since the design variable of the method is set to the density of each element. Therefore, some technical skills are needed to give features of the level-set method to the reaction-diffusion equation based method. The double-well potential function can be a solution of the problem. By the adding double well potential function term, it can push the sensitivity of boundary area to 0 or 1, so that the modified topology optimization gets the features of level-set method [11, 12].

The surface plasmon effect has been used for improving efficiency of thin film solar cell by inserting Ag nano-particles and the shape and size of Ag nano particles were determined for amplifying the surface plasmon effect. This study uses the reaction-diffusion equation based level set method combined with double-well potential functions for deciding the shape and size of nano-particles.

2. Parameter optimization

The level-set method based on the reaction-diffusion equation can give reliable design of structure. However, optimal design of the level-set method is dependent on initial design of the structure. Therefore, it is required to perform the parameter optimization process to decide the prototype model for the application of the level set method.

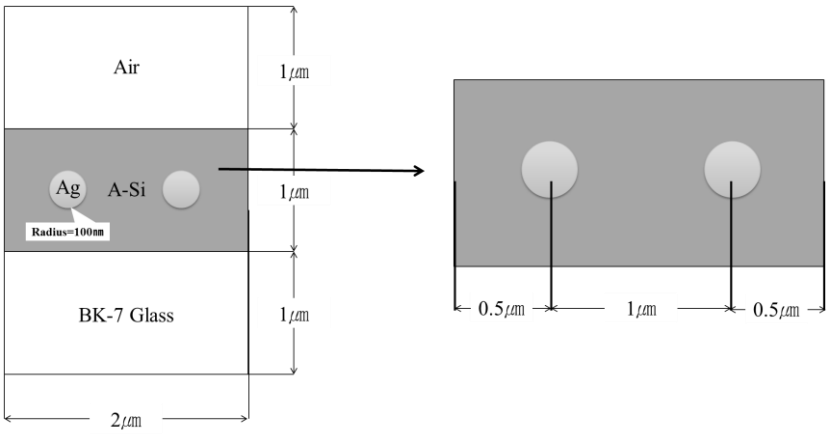

Figure 1: Structure of initial model for parameter optimization

Figure 1 shows that very initial model of the unit structure of thin film solar cells composed of three materials. Top layer of the model is composed of air to describe the incident light environment. Second layer is composed of amorphous silicon to play role as the absorbing layer of a thin film solar cell. Ag nano-particles were arranged in a single array at the second layer to get homogeneity of the absorbing layer. Bottom layer is composed of glass and its role is the substrate of the thin film solar cell. The thickness of each layer is 1μm and the width of all layers is set to 2 μm. Optical properties of material were determined according to the incident light wavelength.

Equation (1) expresses the Helmholtz's equation used as the governing equation for the analysis. The Helmholtz's equation is a kind of modified wave equation which has time-harmonic terms to make the equation be time independent. In the numerical simulation of the thin film solar cell, the equation is used as governing equation for minimizing time variation influence and checking the influence of material properties.

$$\nabla^2 \mathbf{H} + \mu\omega^2 \varepsilon \mathbf{H} = 0 \tag{1}$$

where **H** is the magnetic field strength and ω represents the fixed excitation frequency. ε and μ represent the electric permittivity and the magnetic permeability, respectively.

The objective function expressed in Eq. (2) represents the Poynting vector of the absorbing layer divided by the absorbing layer area. The Poynitng vector means the directional energy flux density. If the vector value is increased, the density of electric field may be increased. It gives the opportunity which makes the thin film solar cell absorb more light. As a result, the efficiency of thin film solar cell will be improved.

$$\frac{\int_{\Omega} \mathrm{Re}\left[\frac{1}{2}\frac{1}{j\omega\varepsilon_0}\left\{\left(\frac{1}{\varepsilon_r}\frac{\partial H_z}{\partial x}H_z^*\right)\hat{\mathbf{x}}+\left(\frac{1}{\varepsilon_r}\frac{\partial H_z}{\partial y}H_z^*\right)\hat{\mathbf{y}}\right\}\right]d\Omega}{\text{Area of absorbing layer}} \tag{2}$$

where H_z* represents the complex conjugate of H_z. Since the transverse magnetic (TM) mode in two-dimensional case is considered, only H_z is taken into account.

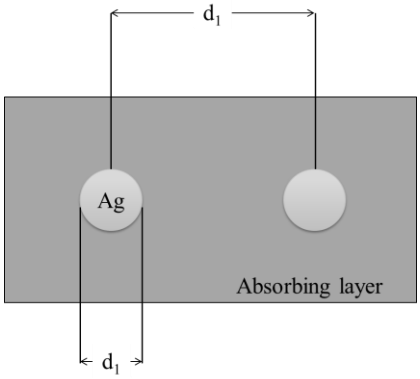

Figure 2: Design variable set-up for parameter optimization

Figure 2 shows that design variables for the parameter optimization procedure. There are two variables which define the interval and the radius of Ag nano-particles. Neumann boundary conditions are applied and periodic boundary conditions are applied to boundaries at both ends. Because only two design variables are considered, a full-factorial orthogonal array which performs optimizing process in all cases is chosen. The interval of Ag nano-particles is divided into 11 levels and the radius of the particles is divided into 10 levels. Therefore, there are 110 cases performed in the parameter optimization process using the full-factorial orthogonal array.

As a result, we can get optimal parameter design of Ag nano-particles in the thin film solar cell. The interval of silver nano particles is determined as 1 μm and the radius of silver nano particles is 70nm. The Poynting vector value of the absorbing layer increased about 10 times larger compared to the initial model.

3. Topology optimization

Based on the model determined by the parameter optimization process, we have designed the optimal shape of Ag nano-particles in the absorbing area by using the level-set method. The objective function, boundary conditions and the governing equation defined during the parameter optimization process are commonly used in topology optimization. The updating scheme and the sensitivity analysis are added for topology optimization.

The reaction-diffusion equation is appropriate to represent a change of phase change and used the equation as an updating scheme. In the proposed method, the reaction-diffusion equation in Eq. (3) is used in this study.

$$\frac{\partial\phi(\mathbf{x},t)}{\partial t} = \varepsilon\nabla^2\phi(\mathbf{x},t) - \frac{\partial\bar{F}(\phi,H_z)}{\partial\phi} \text{ in } \mathbf{x}\in\Omega, \quad 0<t\le T \tag{3}$$

Where Ω is a design domain and ϕ is a density of each element. Eq. (4) represents the sensitivity value using the augment Lagrangian $\bar{F}$.

$$\frac{\partial\bar{F}(\phi,\mathbf{u},\lambda)}{\partial\phi} = \frac{\partial F(\phi,\mathbf{u})}{\partial\phi} + \frac{\partial\hat{G}(\phi)}{\partial\phi}[\lambda + r\hat{G}(\phi)] \tag{4}$$

Where F is the design objective function and $\hat{G}$ is the modified constraint function [11]. However, topology optimization based on the reaction-diffusion equation proposed by Choi et al. [11] may not be regarded as a level-set method since it does not have an interface tracking property. In this study, a technical skill is used in

sensitivity analysis by adding double well potential term and this technical skill make topology optimization based on reaction-diffusion equation have the features of the level set method.

$$g(\phi)=\phi^2(1-\phi)^2,\ p(\phi)=\phi^3\left(6\phi^2-15\phi+10\right) \tag{5}$$

$$\frac{\partial \bar{F}}{\partial \phi}=ag'(\phi)+p'(\phi)\left[\xi\frac{\partial F(\phi,\mathbf{u})}{\partial \phi}+\frac{\partial \hat{G}(\phi)}{\partial \phi}[\lambda+r\hat{G}(\phi)]\right] \tag{6}$$

Eq. (5) expresses double-well potential functions used and Eq. (6) is the sensitivity of the augment Lagrangian combined with double-well potential functions. Double-well potential functions added in the sensitivity of the objective function makes the sensitivity of boundary area to be 0 or 1. The modification separates the boundary between solid and void element clearly. Therefore, phase change can be occurred only at the area of boundary and the optimization process has the interface tracking property. In other words, the sensitivity analysis modified by double-well potential functions makes topology optimization based on the reaction-diffusion equation be regarded as a level set method. In this study, the optimal design of Ag nano-particles was obtained by using topology optimization based on the reaction-diffusion equation combined with double-well potential functions.

4. Numerical results

There are two factors influencing optimal design results in the reaction-diffusion equation based topology optimization. Those are the diffusivity coefficient and the volume fraction constraint. The diffusivity coefficient determines how complex optimal design is and the volume fraction is a constraint condition which limits the total volume of optimal design. We have changed those two factors and checked the influence on optimal design results.

4.1. Variation of the diffusivity coefficient

Beginning from the initial design suggested by the parameter optimization process, optimizations were performed according to three different values of the diffusivity coefficient as 1e-4, 1e-5 and 1e-6. Figure 3 shows optimal shape variations according to different values and Fig. 4 shows the electric field distribution of the absorbing layer. Results indicate that the case of diffusivity as 1e-4 gives the best performance on the basis of the objective value. When the objective value of initial design normalized as 1, the objective value of 1e-4 diffusivity case is 2.31. However, the optimal shape of the best performance is not feasible since the shape is more like two separated particles rather than one particle. Also, the case of diffusivity 1e-6 shows a complex structure of nano-particle such as twigs. Therefore, in terms of the objective value and the feasibility, the case of diffusivity 1e-5 was chosen for an appropriate diffusivity coefficient in the optimization process which has the objective value 1.96. The cases of diffusivity 1e-2 and 1e-3 are excluded since shapes of nano-particle are not clearly distinct.

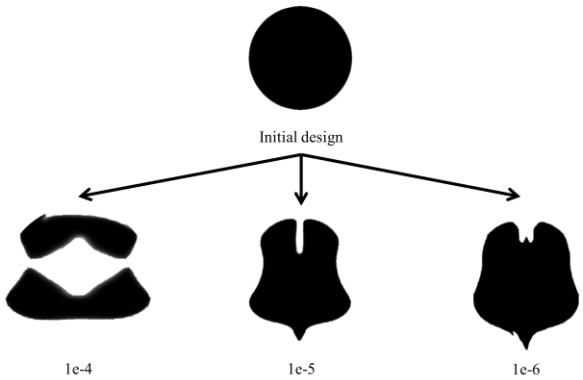

Figure 3: Resultant shapes about diffusivity coefficient variation

4.2. Variation of volume fraction

In this section, the variations of optimal shape and objective value according to volume fraction are obtained. Design domain of initial design is composed of void (amorphous silicon) part and solid (Ag) part. The radius of solid part is 50nm and thickness of outer ring is 50nm. And optimizations were conducted using the every volume fraction whose step size is 0.1 Figure 5 shows that the variation of optimal design and objective value according to each volume fractions. Considering the complexity of shape and objective value, cases of volume fraction 0.6 and 0.7 can be a feasible design. It is noteworthy that higher value of the volume fraction does not guarantee the higher objective value and the optimal shape of Ag nano-particle is sensitive to the initial material distribution.

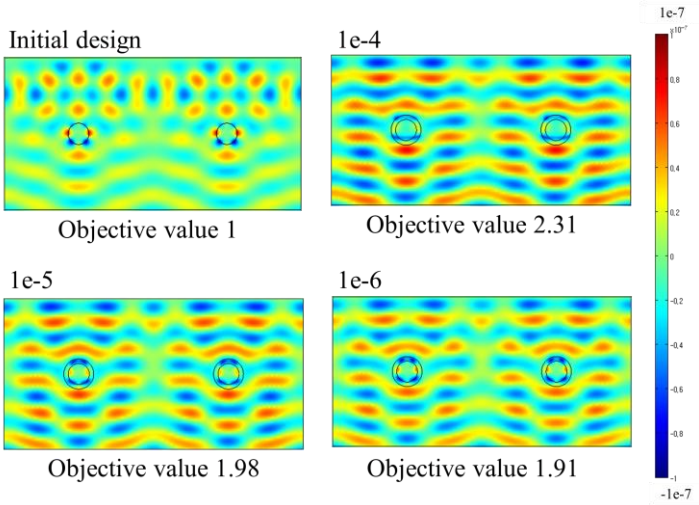

Figure 4: Electric field contour of the absorbing layer after optimization

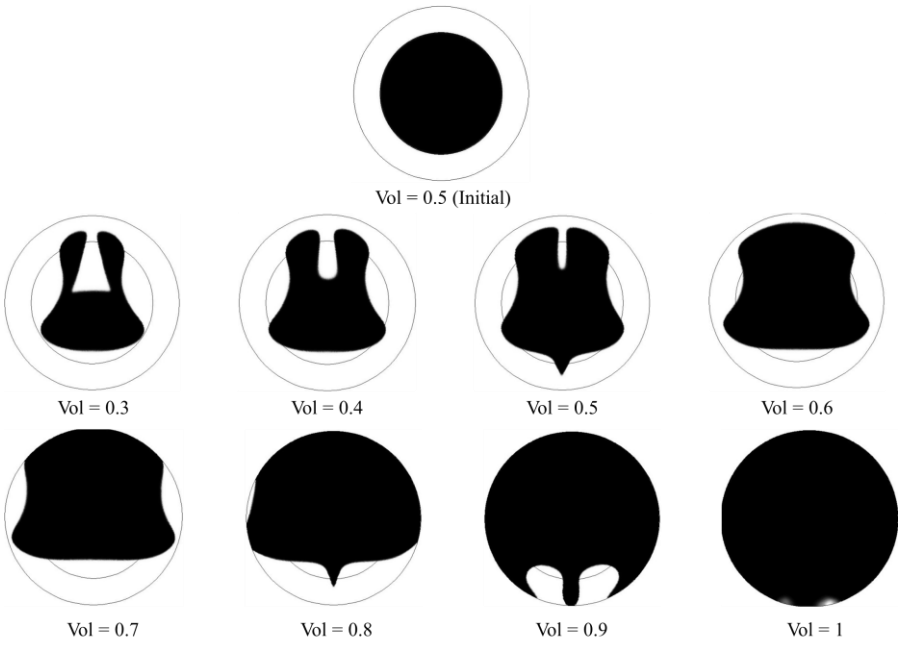

Figure 5: Shape variation according to different volume fraction constraints

Optimal values of the diffusivity coefficient and the volume fraction are determined through results displayed in the Figs. 3~5. Optimal design of Ag nano-particles is suggested when the diffusivity coefficient is 1e-5 with the volume fraction of 0.7. Figure 6 shows that optimal shape and local electric field distribution. The Poynting vector of absorbing layer in optimal design is 1.362e-25 W/m^2. The objective value is increased about 2.5 times compared with that of the initial design.

5. Conclusion

In this study, we have designed an optimal shape of Ag nano-particles in the absorbing layer of a thin film solar cell using topology optimization based on the reaction-diffusion equation combined with double well potential functions. Through deciding the optimal shape of Ag nano-particles, the Poynting vector of the absorbing layer is increased by generating the surface plasmon effect and the efficiency of thin film solar cell is improved as a result. Of course, the improvement of poynting vector is not directly related to the efficiency increase of the thin film

solar cell. However, optimization conducted in this study shows a possibility that the efficiency of thin film solar cell can be improved by adopting the optimization design process. From the topology optimization point of view, the optimizing process used is a level set method which has an interface tracking property. Therefore, we can get an optimal design which has clear boundaries. In conclusion, we have confirmed that topology optimization based on reaction-diffusion equation combined with double well potential functions helps to decide the optimal shape of metal nano-particles.

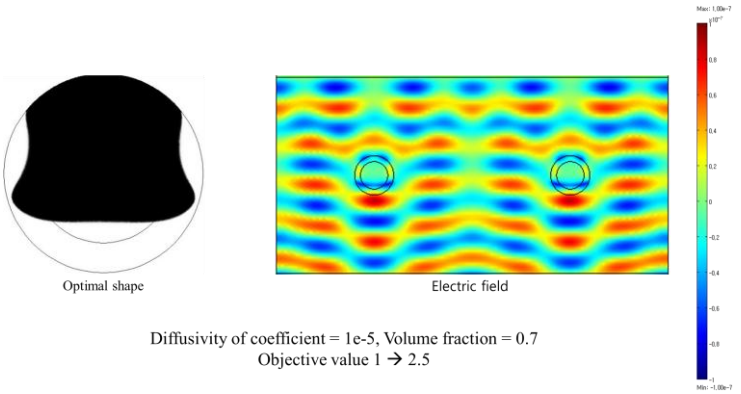

Figure 6: Suggested optimal design of Ag nano-particles in the absorbing layer

6. Acknowledgment
This work was supported by National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (No. 2012-0005701).

7. References

[1] M. A. Garcia, Corrigendum: Surface plasmons in metallic nanoparticles: fundamentals and applications, *Journal of Physics*, 44, 28300101-28300120, 2011.
[2] M. Yang, J. Li, F. Lin and X. Zhu, Absorption Enhancements in Plasmonic Solar Cells Coated with Metallic Nanoparticles, *Plasmonics*, 2013.
[3] F. Tsai, J. Wang, J. Huang, T. Kiang and C. C. Yang, Absorption enhancement of an amorphous Si solar cell through surface plasmon-induced scattering with metal nanoparticles, *Optical Express*, 18(S2), A207-A220, 2010.
[4] C. Sun, H. Gao, R, Shi, C. Li and C. Du, Design Method for Light Absorption Enhancement in Ultra-Thin Film Organic Solar Cells with Metallic Nanoparticles, *Plasmonics*, 2012
[5] A. Feltrin, T. Meguro, M. Ichikawa, F. Sezaki and K. Yamamoto, Light scattering and parasitic absorption in thin film silicon solar cells containing metal nanoparticles, *Journal of Photonics for Energy*, 1, 0170031-0170038, 2011.
[6] S. Pillai, K. R. Catchpole, T. Trupke and M. A. Green, Surface plasmon enhanced silicon solar cells, *Journal of Applied Physics*, 101(9), 0931051-0931058, 2007.
[7] S. Kim, S. Na, J. Jo, D. Kim and Y. Nah, Plasmon enhanced performance of organic solar cells using electrodeposited Ag nanoparticles, *Journal of Applied Physics*, 93(7), 0733071-0733073, 2008.
[8] Y. Akimov and W. Koh, Design of Plasmonic Nanoparticles for Efficient Subwavelength Light Trapping in Thin-Film Solar Cells, *Plasmonics*, 6, 155-161, 2011.
[9] Y. Akimov, K. Ostrikov and E. P. Li, Surface Plasmon Enhancement of Optical Absorption in Thin-Film Silicon Solar Cells, *Plasmonics*, 4, 107-113, 2009.
[10] K. Kelly, E. Coronado, L. Zhao and G. C. Schatz, The optical Properties of Metal Nanoparticles: The Influence of Size, Shape, and Dielectric Environment, *Journal of Physics and Chemistry*, 107, 668-677, 2003.
[11] J. Choi, T. Yamada, K. Izui, S. Nishiwaki and J. Yoo, Topology optimization using a reaction-diffusion equation, *Computer Methods in Applied Mechanics and Engineering*, 200(29-32), 2408-2420, 2011.
[12] A. Takezawa, S. Nishiwaki and M. Kitamura, Shape and topology optimization based on the phase field method and sensitivity analysis, *Journal of Computational Physics*, 229, 2697-2718, 2010.
[13] X. Chen, B. Jia, J. K. Saha, B. Cai, N. Stokes, Q. Qiao, Y. Wang, Z. Shi and M. Gu, Broadband Enhancement in Thin-Film Amorphous Silicon Solar Cells Enabled by Nucleated Silver Nanoparticles, *Nano Letters*, 12(5), 2187-2192, 2012.
[14] J. Zhu, Y. Ren, S. Zhao and J. Zhao, The effect of inserted gold nanosphere on the local field enhancement of

gold nanoshell, *Materials Chemistry and Physics*, 133, 1060-1065, 2012.
[15] W. Liu, X. Wang, Y. Li, Z. Geng, F. Yang and J. Li, Surface plasmon enhanced GaAs thin film solar cells, *Solar Energy Materials and Solar Cells*, 95(2), 693-698, 2011.
[16] H. Mertens, J. Verhoeven, A. Polman and F.D. Tichelaar, Infrared surface plasmons in two-dimensional silver nanoparticle arrays in silicon, *Applied Physics Letters*, 85(8), 1317-1319, 2004.
[17] M.P. Bendsoe and N. Kikuchi, Generating optimal topologies in structural design using a homogenization method, *Computer Methods in Applied Mechanics and Engineering*, 71, 197-224, 1988.
[18] M.P. Bendsoe and O. Sigmund, *Topology Optimization: Theory, Methods and Applications*, Springer-Verlag, Berlin, 2003.
[19] A. Diaz and O. Sigmund, Checkerboard patterns in layout optimization, *Structural optimization*, 10(1), 40-45, 1995.
[20] J. A. Serhian and A. Wiegmann, Structural boundary design via level-set and immersed interface method, *Journal of Computational Physics*, 163, 489-528, 2000.
[21] M. Y. Wang, X. Wang and D. Guo, A level set method for structural topology optimization, *Computer Methods in Applied Mechanics and Engineering*, 192, 227-246, 2000.
[22] T. Yamada, K. Izui, S. Nishiwaki and A. Takezawa, A topology optimization method based on the level set method incorporating a fictitious energy, *Computer Methods in Applied Mechanics and Engineering*, 199 (45-48) 2876–2891, 2010.