COMSOL을 이용한 전자기장 내 나노 스케일 구조물의 설계

(Nano-scale Structure Design in EM fields using COMSOL)

COMSOL Conference Seoul 2012: Nov. 23rd (Fri)

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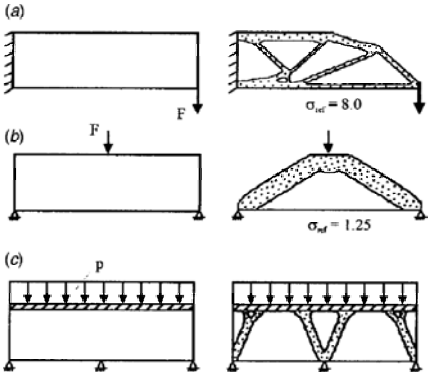
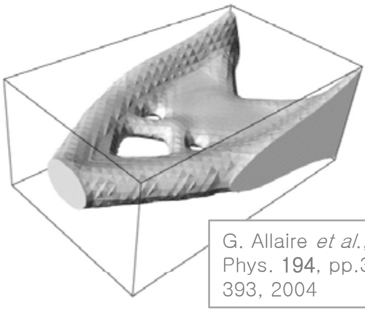
OUTLINE

- **Research Overview**
- **Background of the Study:**
  Topology Optimization in Magneto-static Field
- **Applications:**
  SPR Sensor Design
  Nano-aperture Design
- **Conclusions**

Examples of topology optimization

- Elastic structure





G. Allaire *et al.*, J. Comput. Phys. 194, pp.363–393, 2004

- Magneto-static structure

✓BLDC motor

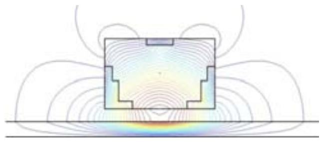
C–H. Im et al., IEEE Trans. Mag., 39, pp.2163–2169, 2003

✓Magneto-strictive sensor

S. H. Cho, Y. Kim, Y. Y. Kim, Sensor and Actuators A, 107, pp.225–232, 2005

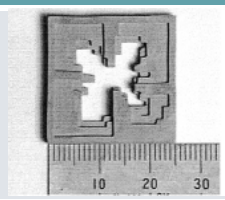
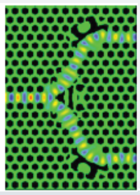
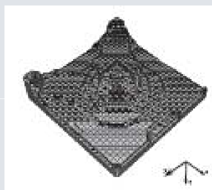
✓Simultaneous design

J. S. Choi, J. Yoo, Comput. Methods Appl. Mech. Engrg, **198**, pp. 2111-2121, 2010



Research Overview

Motivation (1)

Authors	Year	Issues	Design Results
G. Kiziltas *et al.*	2003	Substrate design of a patch antenna (dielectric substrate)	Layered substrate design and Fabrication 
J. Jensen & O. Sigmund	2004	Photonic crystal waveguide design	Topology application to waveguide design  
T. Nomura *et al.*	2007	3D substrate design of a patch antenna	3D topology optimization combined with finite difference method 

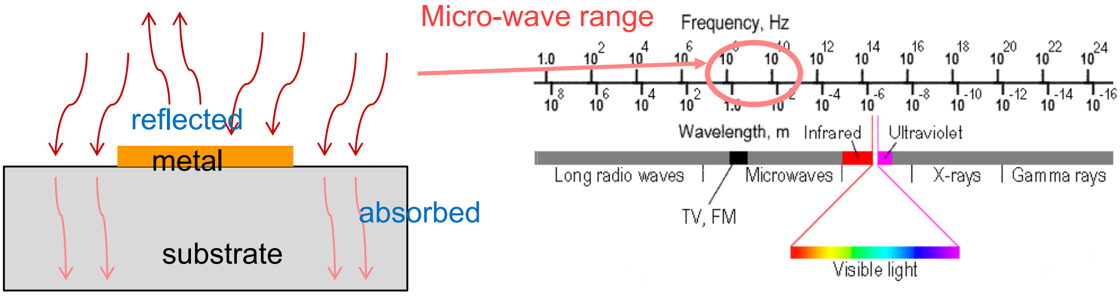
Motivation (2)

- Limitation of the previous works

→ Applied only for substrate parts, that is, Si based material

Reason?

Electromagnetic wave cannot be absorbed into metal for some specific frequency range



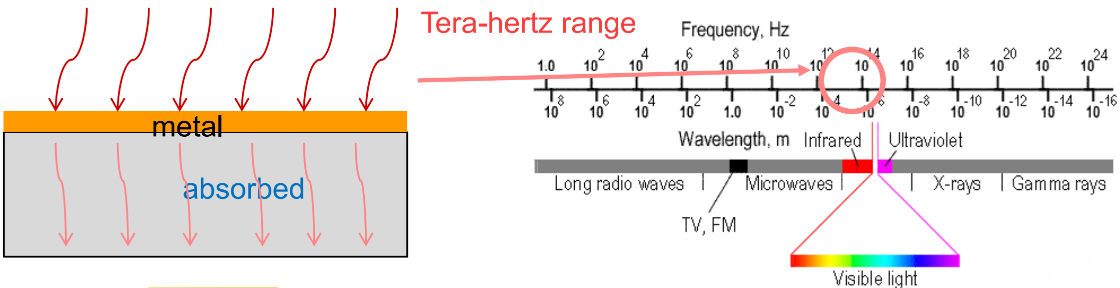
❖ For topology method application, energy must be able to be computed in the design domain.

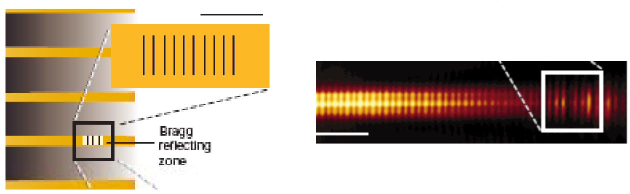
Motivation (3)

- Then, why visible/near infrared frequency range in nano-scale structure?

→ The wave can penetrate into some thin, specific material, so topology optimization may be applied.

→ Many prospective application using the surface plasmon polariton (SPP) effect.



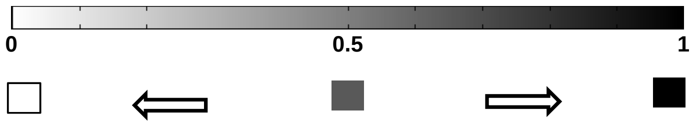


W. L. Barnes *et al.*, Nature, 424, pp.824-830, 2003

Topology Optimization Method (1)

Solid Isotropic Material with Penalization (SIMP)

Void $E^e_{ijkl}(x) = \rho \overline{E}_{ijkl}$ Filled Material

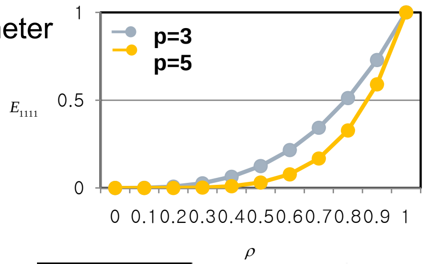


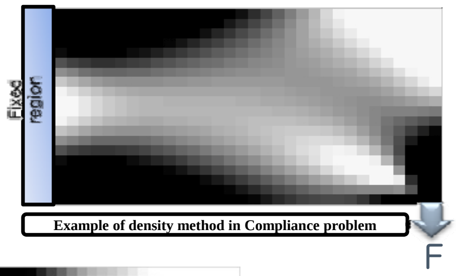
Penalization parameter

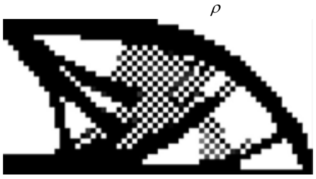
$$E^e_{ijkl}(x) = X(x)\overline{E}_{ijkl}$$

$$E_{ijkl} = \rho \overline{E}_{ijkl}$$

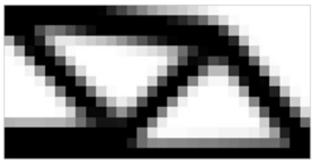
$$E_{ijkl} = \rho^p \overline{E}_{ijkl}$$







Without filtering



Filtering

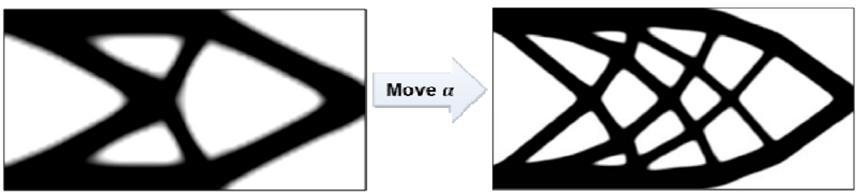
Topology Optimization Method (2)

Reaction – Diffusion Equation Based method

$$\begin{cases} \dfrac{\partial \phi(t)}{\partial t} = \alpha \nabla^2 \phi(t) - \dfrac{\partial \overline{f}(\phi)}{\partial \phi} \quad in \quad \Omega_T := \Omega \times (0,T) \\ \dfrac{\partial \phi(t)}{\partial \hat{\mathbf{n}}} = 0 \quad in \quad \partial\Omega_T := \partial\Omega \times (0,T), \quad 0 \le \rho \le 1 \end{cases}$$

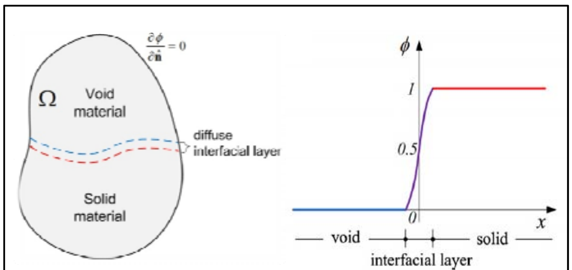
- Diffuse interfacial layer

$$\alpha = \alpha_0 V_{total} = \alpha_0 \int_\Omega dx$$



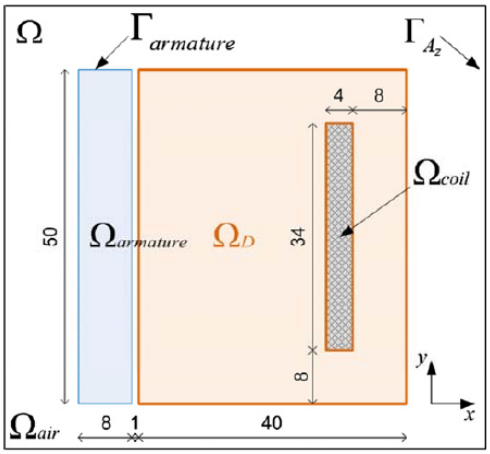
- Reaction term: gradient of the augmented Lagrangian

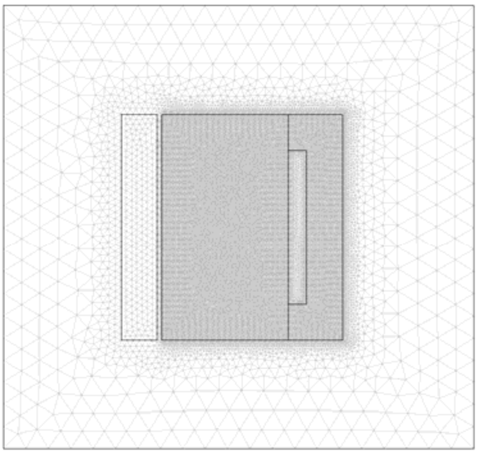
$$R(\phi) = -\frac{\partial \overline{f}}{\partial \phi} = -\frac{\partial f(\phi, A_z)}{\partial \phi} - \frac{\partial g(\phi)}{\partial \phi}[\lambda + rg(\phi)]$$



Separation of material phases

C-core Actuator: Analysis Model (1)





Application modes
AC/DC Module - Quasi-statics, Magnetic - Perpendicular Induction Currents, Vector potential
COMSOL Multi-physics - PDE mode - Optimization and sensitivity

	Number of Element
Air/ Coil/ Armature	126354 [triangle element]
Yoke	56928 [triangle element]

- Core design for a C-core actuator
- Design goal is to maximize the x-directional magnetic force on an armature
- Topology optimization using SIMP method and Reaction Diffusion based method

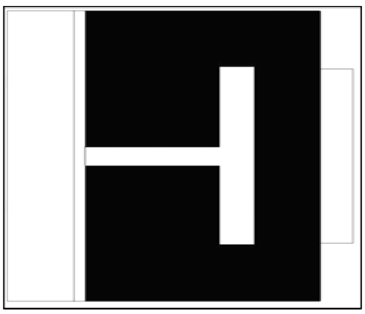
$$\text{Maximize} \quad f(\phi, A_z(\phi)) = -\frac{1}{2\mu_0}\int_{\Gamma_{armature}} \left[\left(B_x^2 - B_y^2\right)n_x + 2B_xB_yn_y\right]dl$$

$$\text{Subject to} \quad g(\phi) = \int_{\Omega_D} \phi dx - V_{req}\int_{\Omega_D} dx = 0$$

$$0 \le \phi \le 1$$

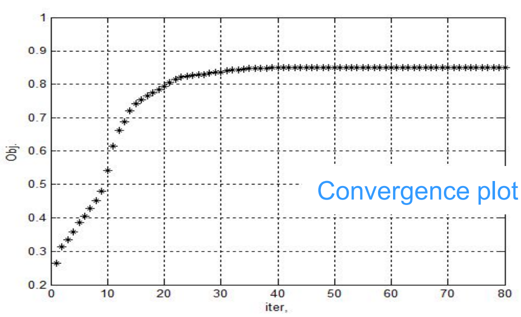
C-core Actuator: Topology Optimization Results (1)

SIMP method

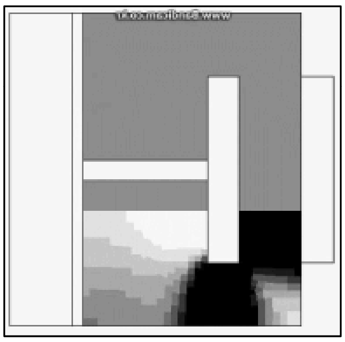


Initial design

Volume fraction = 100 %



- Optimization result

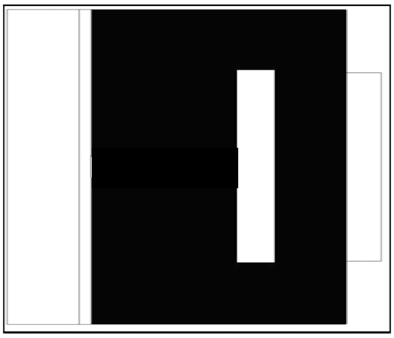


optimal

Volume fraction = 80 %

C-core Actuator: Topology Optimization Results (2)

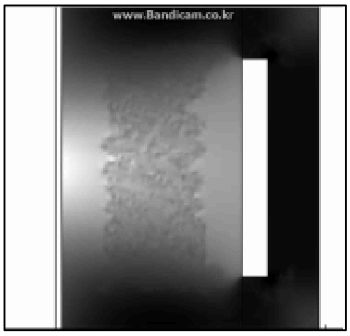
R-D method



Initial design

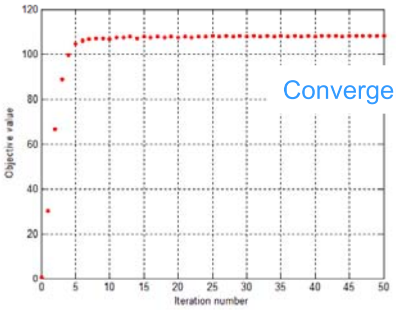
Volume fraction = 100 %

- Optimization result

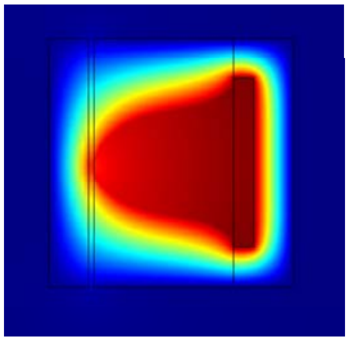


optimal

Volume fraction = 80 %



Convergence plot



Contour of the Magnetic vector Potential A_z

SPR Senor Design - Concept

- Application of topology optimization for the metal part design in a sensor using the surface plasmon polariton effects.

- This is using attenuated total reflectance (ATR). It is a sampling technique used in conjunction with infra-red spectroscopy which enables samples to be examined directly in the liquid or solid state without further preparation.
(*Perkin Elmer Life and Analytical Sciences*. 2005. http://las.perkinelmer.com/content/TechnicalInfo/TCH_FTIRATR.pdf. Retrieved 2007-01-26.)

- Previously, the design has been performed based on the physics theory.

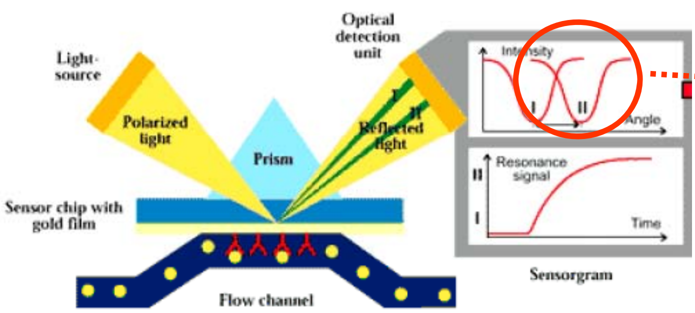
Research Overview

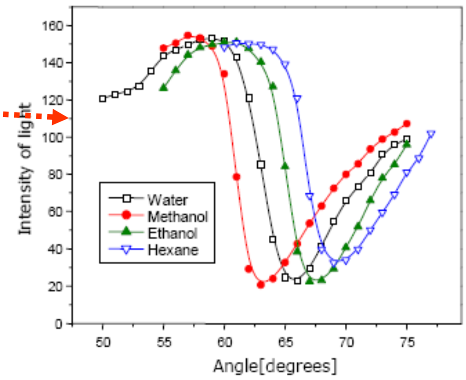
✓ SPR sensing algorithm

- prism or grating structure is necessary for the surface plasmon effect
- sample is positioned beneath the Au (or Ag) film.

➡ Surface Plasmon Resonance (SPR) angle is changed according to the refractive index of the sample.

Detection of surface molecules





Background: Surface Plasmon Effect

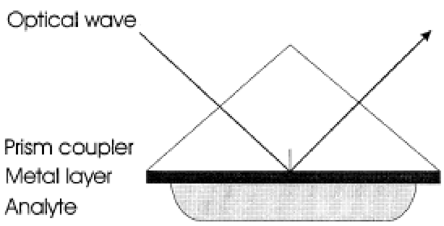
✓ What is Surface Plasmon?

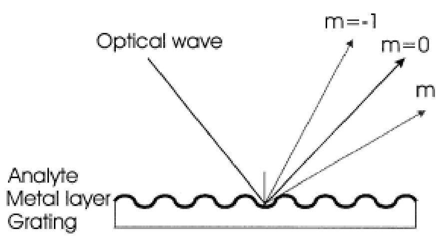
Surface electromagnetic waves: that propagate in a direction parallel to the metal/dielectric (or metal/vacuum) interface

One can use an electron or light beam (visible and infrared are typical). The incoming beam has to match its impulse to that of the plasmon.

➡ propagation constant: $\beta = k\sqrt{\dfrac{\varepsilon_m n_s^2}{\varepsilon_m + n_s^2}}$

k - space wave number
ε_m - dielectric constant of the metal
n_s - reflective index of the dielectric
real of $(\varepsilon_m) < -n_s^2$



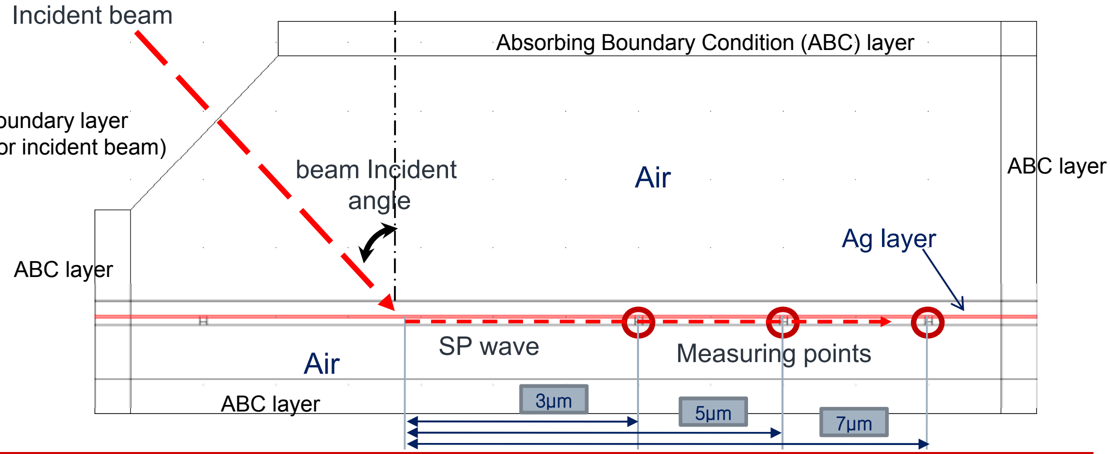


J. Homola et al., Sensors and Actuators B, **54**, pp. 3-15, 1999.

Analysis Model (1)

- Efficiency depends on wavelength, incident angle and Ag thickness.
- Light passes through the air layer and hits the Ag layer and the surface palsmon wave occurs under the layer.
- Grating structure is located on the Ag layer.

➤ Governing Equation: $\frac{\partial}{\partial x}\cdot\left(\varepsilon_r^{-1}\frac{\partial}{\partial x}H_z\right)+\frac{\partial}{\partial y}\cdot\left(\varepsilon_r^{-1}\frac{\partial}{\partial y}H_z\right)-\frac{\omega^2}{c^2}H_z=0$



Analysis Model (2)

➤ Poynting vector

$$P_{output}=\frac{-1}{2\omega\varepsilon_0 L_x}\int_{\Omega_{output}}\Re\left[\frac{i}{\varepsilon_r}\frac{\partial H_z(x,y)}{\partial x}H_z(x,y)\right]dxdy$$

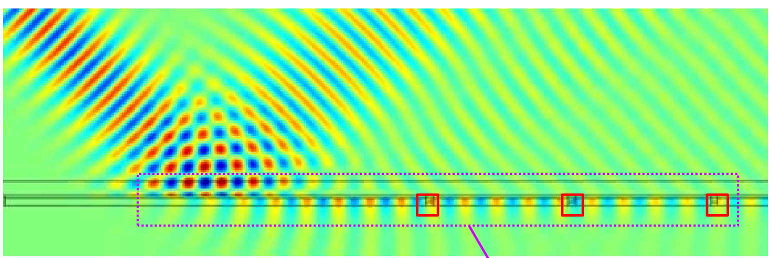
➤ Efficiency

$$\eta=\frac{P_{output}e^{-1}}{\left(1-e^{-1}\right)P_{input}}$$

: computed based on the TM wave

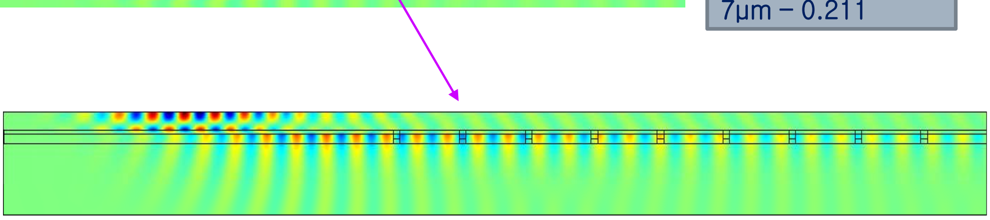
Application modes

COMSOL Multiphysics
- PDE mode
- Optimization and sensitivity



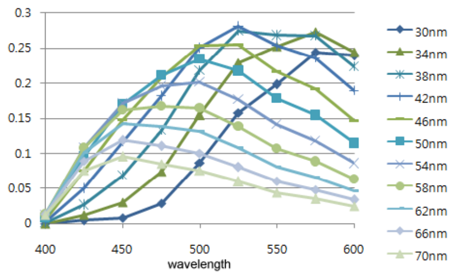
Wave Length – 475nm
Incident Angle – 45deg
Ag Thickness – 50nm

Efficiency
3µm – 0.507
5µm – 0.368
7µm – 0.211

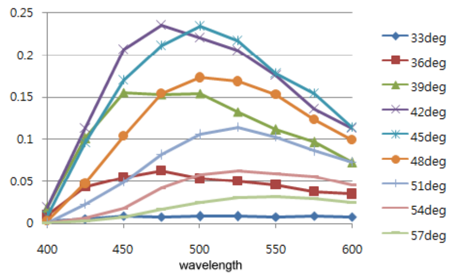


Parameter Study (1)

➢ Efficiency according to wavelength change

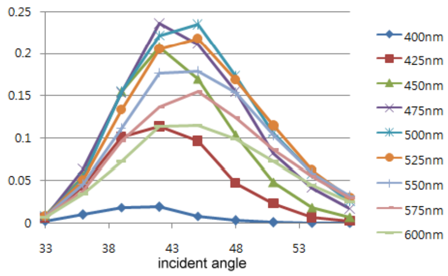


Incident Angel – 45deg

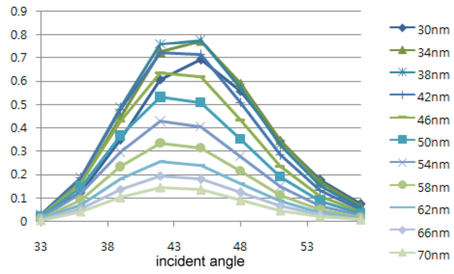


Ag Thickness - 50nm

➢ Efficiency according to incident angle change



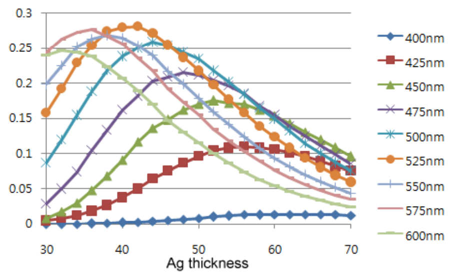
Ag Thickness – 50nm



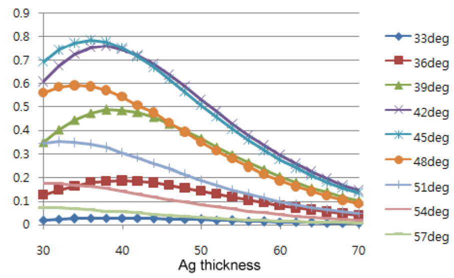
Wave Length – 475nm

Parameter Study (2)

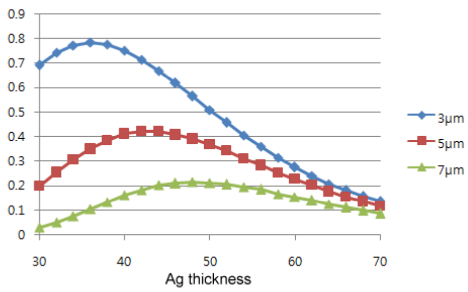
➢ Efficiency according to incident angle change



Incident Angle – 45deg



Wave Length – 475nm



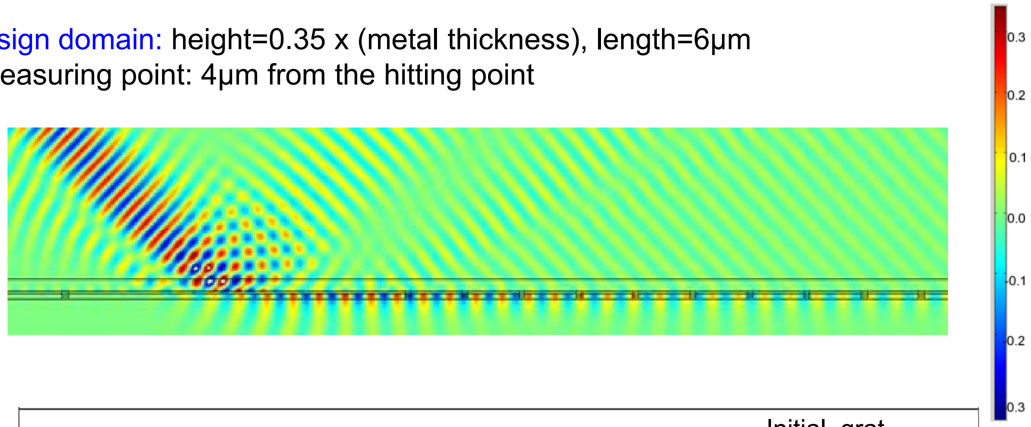
Wave Length – 475nm
Incident Angle – 45deg

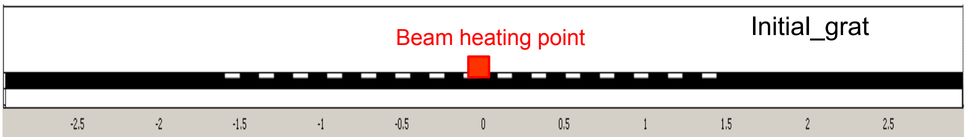
Optimal parameter

Wavelength = 488nm
Angle = 44deg
Ag Thickness = 49nm

Initial Grating Model

Design domain: height=0.35 x (metal thickness), length=6μm
measuring point: 4μm from the hitting point



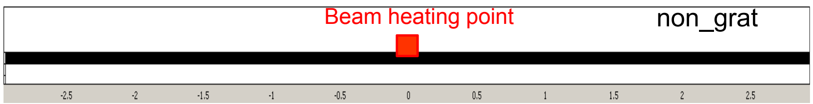


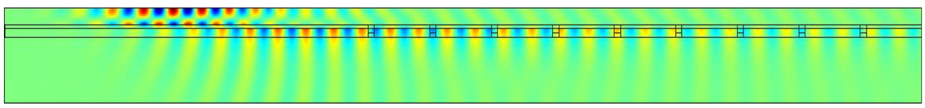
Wavelength = 488nm
Angle = 44deg
Ag Thickness = 49nm

Groove depth = 0.35*T
Groove width = 90nm
Grating period = 210nm

Comparison of Results (1)

Non-grating model
Ag thickness = 49nm

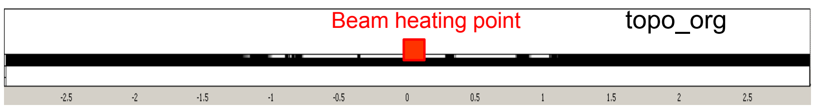


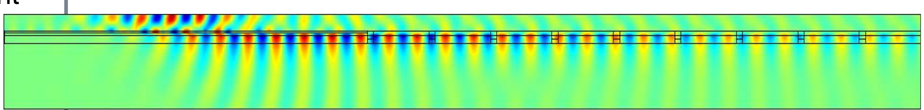


Topology optimization result

- Design domain
  upper 35% of the Ag part
  ±3 μm from the heating point

- Objective function
  maximize $\eta(H_z(\rho))$
  subject to *Boundary Condition*
  $0 < \rho \le 1$

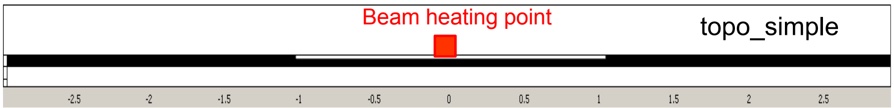


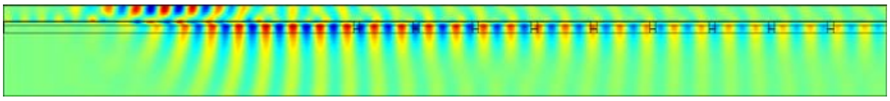


$$n = \rho n_{Ag} + (1-\rho) n_{Air} \quad , \quad n = \sqrt{\varepsilon_r \mu_r}$$

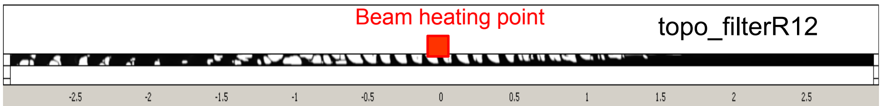
Comparison of Results (2)

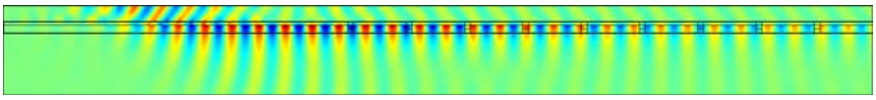
Simplified model of the optimization result



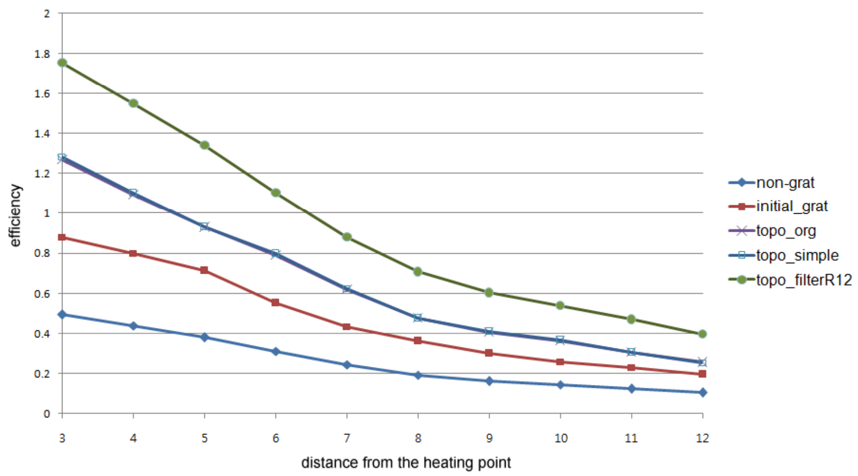


Other Topology optimization result
by filter size change





Comparison of Results & Conclusions

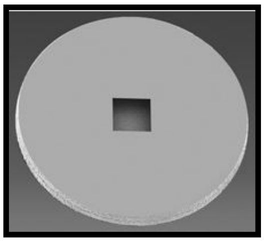


- ✓ Intermediate structures in the original optimization result can be regarded as noise.
  → Thin Ag layer is effective.
- ✓ Grating structure is good to improve performance.
- ✓ Detail design is required considering the manufacturing tolerance.

Conclusions of the SPR Sensor Design

- ✓ Topology optimization scheme may be applied to the design domain composed of metal.
- ✓ However, it is frequency dependent problem, that is, available only for very high frequency range as in visible/near infra-red range.
- ✓ Many prospective applications are expected: (however), tens of percentage improvement may be possible.
- ✓ For the application of microwave (GHz) range, also to overcome some gray scale results, other approaches are necessary.

Research Overview

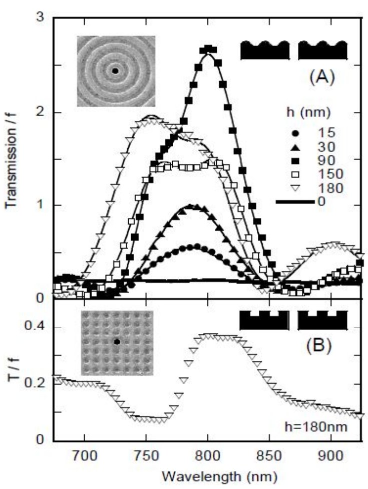


Nano-aperture

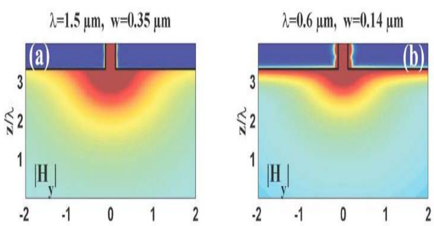
Advantages	Disadvantages
Easy to manufacture	Low transmittance

- The Objective of Study

: Improving Poynting vector under nano-aperture
(Genetic algorithm and ON/OFF method used)



Non-grating



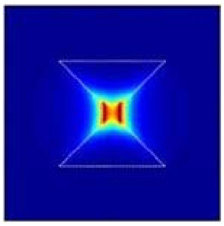
Periodic grating

Previous Works:
Periodic grating or
Non-grating

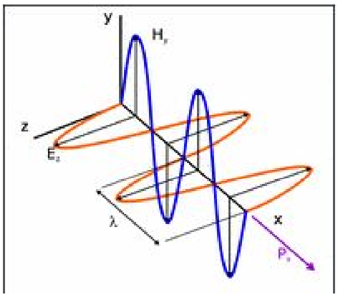
Tineke Thio, K. M. Pellerin and R. A. Linke, Optics Letters, Vol. 26, No. 24, pp. 1972~1974, 2001.
P. Lalanne, J. P. Hugonin and J. C. Rodier, J. Opt. Soc. Am, Vol. 23, No. 7, pp. 1608~1615, 2006.

Research Overview

- Poynting Vector – The energy flux of an electromagnetic field



A bowtie nano-aperture Model



Concept of the Poynting vector

$$\vec{P}\,(\textbf{Poynting vector}) = \vec{\mathbf{E}} \times \vec{\mathbf{H}}$$

- Poynting Vector – The energy flux of an electromagnetic field

$$\nabla \times E = -j\omega\mu H$$
$$\nabla \times H = j\omega\varepsilon E$$

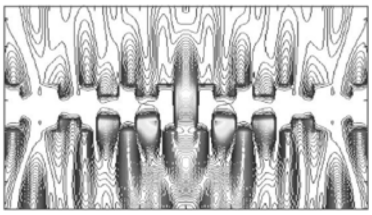
$$P\,(Poynting\ Vector) = Real(E \times H^*)$$

TE mode

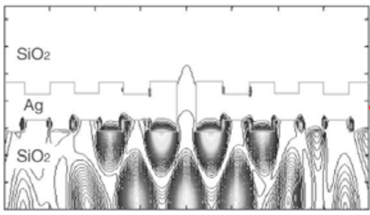
$$\begin{vmatrix} i & j & k \\ E_x & E_y & E_z \\ H_x^* & H_y^* & H_z^* \end{vmatrix} = E_y H_z^* i - E_x H_z^* j$$

Background: Plasmon Effect

- Verification of COMSOL Program

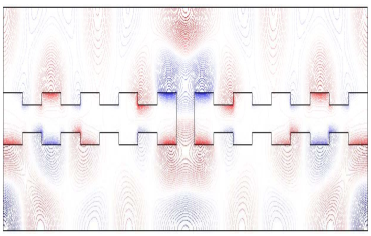


Nano-aperture Grating with 425nm-period

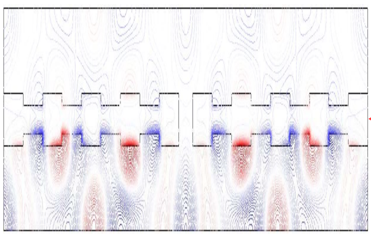


Nano-aperture Grating with 550nm-period

Similar Result!



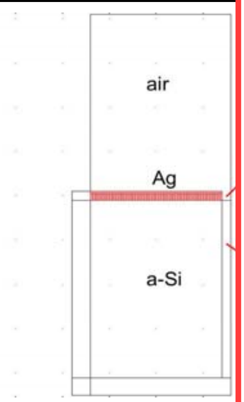
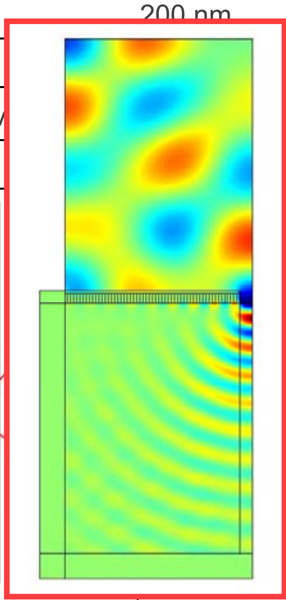
425nm period result with Comsol



550nm period result with Comsol

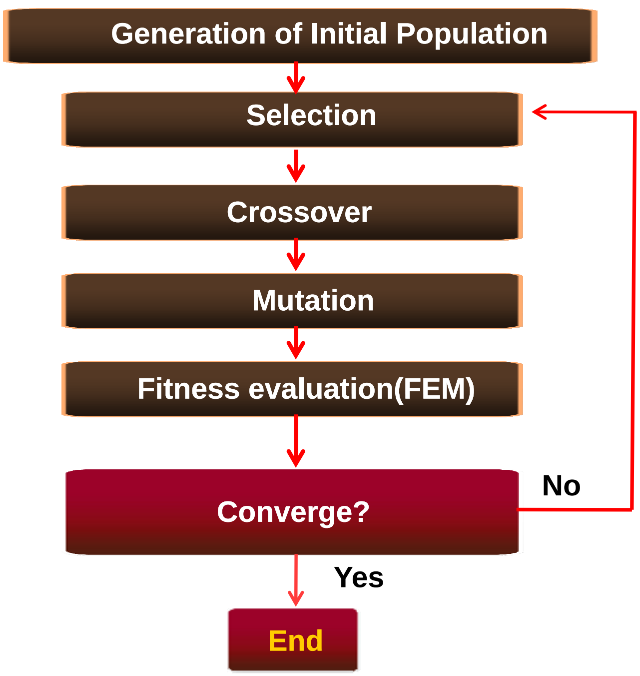
Satoshi Shinada, Jiro Hashizume and Fumio Koyama, Applied Physics Letters , Vol. 83, No. 5, pp. 836-838, 2003

Analysis of the Initial Model

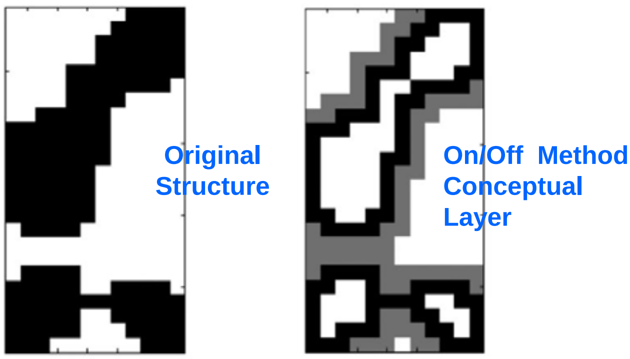
	Specification
Aperture	Ag (Relative permittivity, ε_r = -32.222216+1.727854**i*)
Aperture Length	200 nm
Aperture Thickness	
Substrate	a-Si (Relativ … 21135+0.496388**i*)
Wavelength	
Modeling	 2-D Symmetric Model   …nm+75nm=100nm Design Domain

Optimization Technique

- **Genetic Algorithm Flowchart**



- **ON/OFF Algorithm**



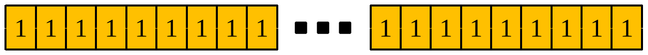
- On/Off Method
- Sensitivity calculation of each element by changing its chromosome (0 → 1, 1 → 0)
  0 → 1
- Less iteration time 1 → 0

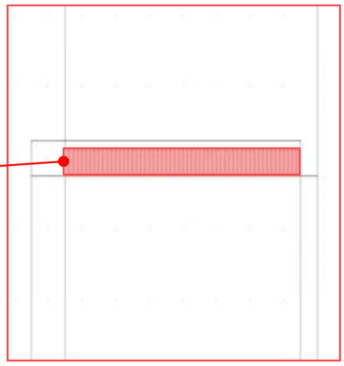
Optimization Process: GA (1)

- **Objective Function**

Maximize Poynting Vector
Volume constraint = 50%

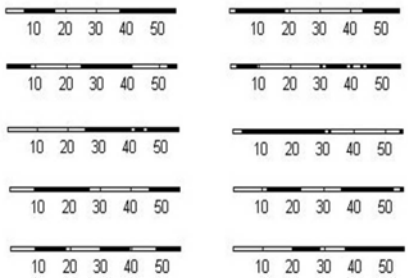
Nano-aperture Grating Domain





GA Design Domain

Mapping of the GA domain to chromosome array(1 or 0)
1 → Material(Metal)
0 → Substrate

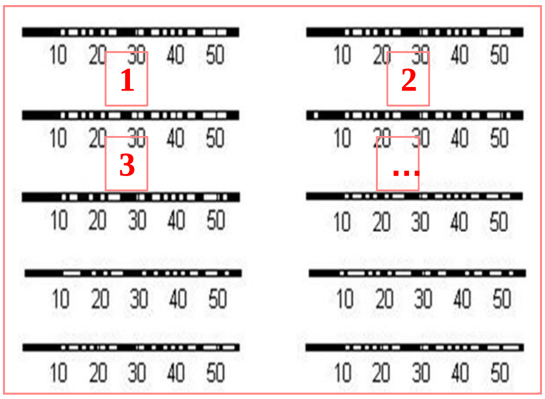


Initial Population

Population – 10 individuals
Selection – Roulette Wheel
Crossover – An offspring inherits genes from parents
Mutation – An offspring gets some genes, which parents doesn't have, in a random process.

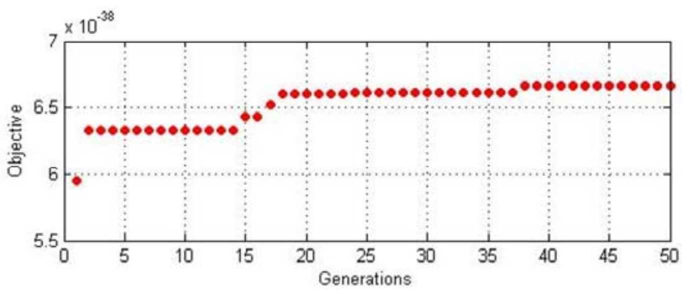
Fitness Function = $\vec{\mathbf{E}} \times \vec{\mathbf{H}}$

Optimization Process: GA (2)



GA Result after 50 Generations

Best shape from the GA



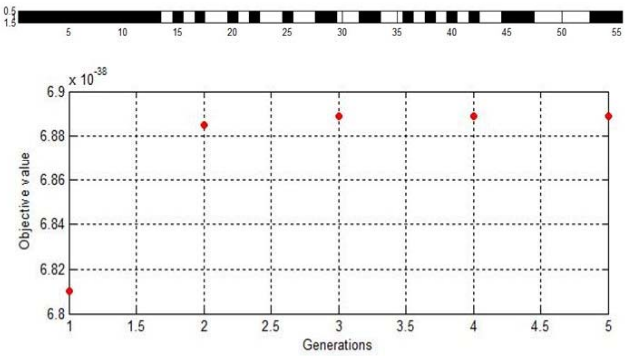
Objective functions Convergence

- GA Result

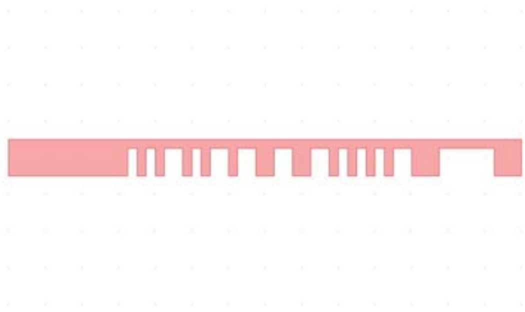
Comsol 3.5 and MATLAB used.
Objective value = 6.6629e-38 (W/m^2)
Normalized Output = 1.1739

Optimization Process: ON/OFF

- **ON/OFF Method Result**



On/off Result after 50 Generations of the GA



Optimal Nano-aperture Shape

- ON/OFF method application based on GA based result
- On/off method for whole design domain
- Objective value = 6.8887e-38 (W/m^2)
- Normalized Output = 1.2137

Conclusions of the Nano-aperture Design

✓ Initial model has low transmittance. To improve the performance, the genetic algorithm and ON/OFF method are used for optimization.

✓ The output of the optimal shape after GA and ON/OFF application increases about 21%.

✓ Topology optimization based on the reaction-diffusion equation may be applicable for the aperture design.

Conclusions

- COMSOL is effective for analysis and design of the structure in electromagnetic field not only for macro-scale but also for nano-scale.
- Also, it may be combined with several optimization schems to improve the system performance.
- Many prospective applications are expected: (however), tens of percentage improvement may be possible.

Prospective Future Applications

- Application of the structure design for 3D cases
  → Is the analysis result reliable?
- Meta-material design for negative permeability as well as negative permittivity
  → Frequency dependent problem: Is geometric change by topology optimization enough?

Thank you