Optimal Design for the Grating Coupler of Surface Plamons

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Abstract: We present an optimization procedure to optimize the maximum coupling of free space optical wave to surface plasmon.. Shape derivative from shape sensitivity analysis is calculated, and the corresponding partial derivatives of the objective functional with respect to finite number of design variables are derived. Even though only a local optimal configuration for a given initial condition is obtained due to the complexity of the problem, the objective functional converges rapidly to a near optimal one.

Keywords: optimal design, surface plasmon, grating coupler

1. Introduction

Surface plasmons [1] are alternating currents propagating along the interface between metal and dielectrics as shown in Figure 1. The plasmonic wave generated has the remarkable property of x-ray wavelength but only optical frequency. For this reason, the energy focused from photon in free space to sub-wavelength dimensions can be used in a variety of applications in nanoscale technology, including Heat Assisted Magnetic Recording (HAMR), nanolithography, and communications among computer.

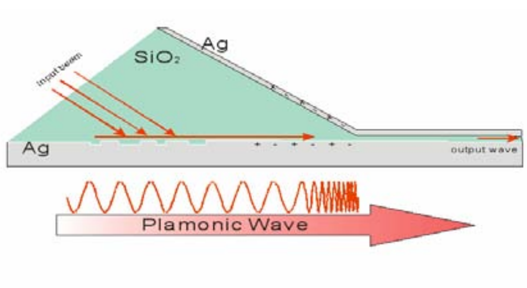

Figure 1. Surface plasmonic wave excited along the interface between metal and dielectrics.

It can be show that time harmonic wave propagates along the interface, while decaying exponentially away from the interface. In the Transverse Magnetic mode, the whole electromagnetic field is characterized by one single variable $H_z(x,y)$, the magnetic field in z direction and defined on x-y plane. The surface wave has the following form

$$H_z(x,y) = \begin{cases} Ae^{-k_d y - jk_{sp}x}, & y>0 \\ Ae^{k_m y - jk_{sp}x}, & y<0 \end{cases} \qquad (1)$$

where x is the direction of propagation of the wave, $j^2=-1$, and the constants k_d, k_m and k_{sp} are related by

$$k_{sp} = \sqrt{\frac{\epsilon_m(\omega)\epsilon_d(\omega)}{\epsilon_m(\omega)+\epsilon_d(\omega)}}k_0$$

$$k_{sp}^2 = k_0^2 + \frac{k_m^2}{\epsilon_m} = k_0^2 + \frac{k_d^2}{\epsilon_d}$$

Here $\varepsilon_m(\omega)$, $\varepsilon_d(\omega)$ are the relative dielectric constant of metal and the dielectrics and k_0 is the wave number in free space. Therefore a necessary condition for the excitation of surface plasmon is $0<\varepsilon_d<-\varepsilon_m$.

In this paper, the problem of designing an efficient grating coupler which generates surface plasmons from free space optical waves is considered. The design variable is the interface profile between the metal (Ag) and dielectrics (SiO_2) and here we only consider the geometry with finite number of gratings. The same problem is tackled with a different approach in [2], however the sequential optimization procedure used there is only near optimal. Here, using the state-of-the-art theory developed in shape analysis, we derive the relation, called the shape derivative, between the change of the profile and that of the objective function (defined to be the output coupled energy along the interface). Then a gradient ascent approach is applied to find the optimal grating coupler.

2. Mathematical Formulation of the design problem

For a given input beam of photon, the amount of energy coupled into the surface wave can be characterized as the Poynting vector along a surface (a line in 2D our geometry) Γ. In another word, we want to design a grating coupler for the following optimization problem

$$\max \quad J(\Omega, H_z(\Omega)) = \frac{1}{2}\int_\Gamma \mathrm{Re}(\vec{E}\times\vec{H}^*)\cdot\vec{n}ds \quad (2)$$

where Ω is the geometry (the position of the gratings) we want to optimize. Using the fact that all the field quantities can be written as a function of H_z only, the above objective functional can be simplified as

$$J = \int_\Gamma \mathrm{Re}\left(\frac{1}{\epsilon_r}\right)|H_z|^2 ds \qquad (3)$$

Here the magnetic field H_z satisfies the following Helmholtz equation

$$\nabla\cdot\left(\frac{1}{\epsilon_r}\nabla H_z\right) + k_0^2 H_z = 0 \qquad (4)$$

The relative dielectric constant ε_r is either ε_m or ε_d, depending on the domain. We concentrate mainly on gratings that are characterized by a few discrete variables (x_i's,h_i's) as in Figure 2, even though shape sensitivity analysis in next section can be applied to arbitrary geometry.

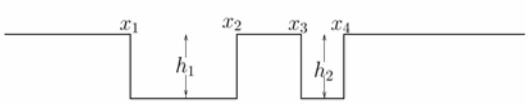

Figure 2. The design variables that characterize the geometry of the problem.

3. Shape Sensitivity analysis

Since for general shape optimization problem the unknown is a geometric object, there are certain special difficulties associated with it. Firstly, we need to find a way to represent to unknown geometry. In some cases, the geometry may be represented as finite number of discrete variables, or points. However, it is hard to handle topological changes like merging or breaking. Secondly, it is not so straightforward to find the gradient of the objective functional with respect to the design variables, even in cases with finite number of parameters. Up to now, there are two types of methods to treat general shape or topology optimization. The first one is distributed material method [3], in which the material are characterized by a continuous density and extra cares need be taken to restrict the density to be piecewise constant to approximate the real material. The second is to treat the exact geometry, and the boundary of the shape is evolved to optimize the objective functional [4]. Real progress was made starting from the seminal work of Sokolowski and Zolesio [5] [6], in which the domain Ω is interpreted as a dynamic one Ω_t depending on time t. We assume Ω_t is evolved from Ω_0 with some defined velocity V(y,t) on Ω_t, i.e

$$\Omega_t = \left\{ y(x,t) \mid \frac{d}{dt}y(x,t) = V(y(x,t),t),\ y(x,0) = x \in \Omega_0 \right\}$$

The second approach enjoyed many successes in different applications together with other progress made in mathematics [7] [8], and is the one taken in this paper. For any given velocity field, we can calculate the *shape derivative* of the objective function in the direction of the velocity,

$$dJ(\Omega;\vec{V}) = \lim_{t\to 0}\frac{J(\Omega_t) - J(\Omega)}{t} \qquad (5)$$

Following [3], assuming the velocity on the fixed boundary are all zero, then the shape sensitivity is

$$\begin{aligned} dJ(\Omega;\vec{V}) &= \mathrm{Re}\left(\left[\frac{1}{\epsilon_r}\right]\int_{\Gamma_m}\nabla H_z^+\cdot\nabla u^- V_n ds\right) \\ &= \mathrm{Re}\left(\left[\frac{1}{\epsilon_r}\right]\int_{\Gamma_m}\nabla H_z^+\cdot\nabla u^- V_n ds\right) \quad (6) \end{aligned}$$

Here Γ_m is the part of the boundary we want to evolve to optimize the objective functional, which is assumed to be different from Γ, the boundary along which we calculate the objective functional. [x] means the jump of the quantity x across the interface. If there is no jump in the properties in the material or the material is homogeneous, the change of any interior boundary has no effects on the objective functional. The superscript + and – denote the one sided derivative of the gradients in the upper or lower stream direction of the normal vector n on the boundary. V_n is the normal component of the velocity field V and u is the adjoint variable, whose solution satisfies the adjoint equation

$$\nabla \cdot \left(\frac{1}{\epsilon_r}\nabla u\right) + k_0^2 u = \delta_\Gamma \mathrm{Re}\left(\frac{1}{\epsilon_r}\right) H_z^* \qquad (7)$$

The adjoint equation can be interpreted as the Lagrange Multiplier to the constraint governing Helmholtz equation (4) for H_z of the optimization problem. Adjoint equations are employed extensive and essential to facilitate the calculation of shape derivative in shape optimization. However, it is absent from certain applications, like those from structure optimization or symmetric eigenvalue problems, because the governing equation is self-adjoint and the objective functional is a special one, such that the adjoint variable is the same as the solution of the governing equation. For computational convenience, the adjoint variable used here is actually the complex conjugate of the Lagrange Multiplier in the usual sense. Because of the discontinuity in ε_r, the gradient of H_z and u are not continuous across the interface. However, using the boundary condition across the interface, the numerical value from the two formulas are the same as long as we don't choose the one sided gradients of H_z and u from the same sides. The results are also independent on the sign of the normal direction n, since it appears exactly twice as a product.

4. Numerical Methods and results

4.1 Gradients of the objective functional

Once we find the shape derivative, we can get the velocity (actually only the normal direction of the velocity) leading to local minimum or maximum of the objective functional. In current problem, for general geometry, the normal component of the velocity on the boundary to choose to maximize the objective functional is

$$\begin{aligned} V_n &= \mathrm{Re}\left(\left[\frac{1}{\epsilon_r}\right]\nabla H_z^+ \cdot \nabla u^-\right) \\ &= \mathrm{Re}\left(\left[\frac{1}{\epsilon_r}\right]\nabla H_z^- \cdot \nabla u^+\right) \end{aligned} \qquad (8)$$

The geometry can be uniquely determined by moving the boundary points of the interface in the normal direction according to the velocity V_n. In practical engineering design, it turns out that finite gratings determined by a few parameters are sufficient. There may be difficulties fabricating general structures due to the resolution limit of lithography. In this situation, the objective functional is actually $J(x_1, x_2, \ldots, x_N, h_1, h_{2,\ldots,} h_M)$. The gradient of the objective function with respect to these variables can be calculated with the analysis from last section, and are appropriate integrals along the boundary corresponding to that variable. For example, let I be the bottom horizontal boundary of the first grating in Figure 2, the we have

$$\frac{\partial J}{\partial h_1} = \int_I \mathrm{Re}\left(\left[\frac{1}{\epsilon_r}\right]\nabla H_z^+ \cdot \nabla u^-\right) ds \qquad (9)$$

Once we find all the partial derivatives of the objective function, what follows are just standard gradient ascent methods in optimization. Those partial derivatives can also be calculated from finite differences by varying the variables by a small amount. However, the numerical discretization error could be amplified by order of magnitudes, leading to an inaccurate derivative and possible failure of the method.

4.2 Comsol PDE simulation settings

The simulations are performed using COMSOL Multiphysics 3.3 in RF module, in-plane waves in TM mode. The parameters can be found from Table 1 in the appendix, and the computational domain is wrapped by a perfectly matched layer (PLM). An input Gaussian beam is specified on one of the dielectric boundary. To reduce the total computational time and relax the memory requirement, the two governing equations (4) and (7) are solved sequentially. Once H_z is found, we can setup the equation (7) in weak form easily: the left hand coefficient are the same as (4), while the right hand side is just a integral on the boundary Γ in contrast to a domain integral in the usual case. In this way, the total number of mesh points can be twice as large as the maximum of solving two equations simultaneously.

4.3 Numerical results and discussion

Starting with three gratings, assuming all the gratings have the same height, we have seven variables for the problem to optimize. The final optimal grating is shown in Figure 3 and the convergence of the method (number of iterations versus the value of the objective functional) in Figure 4. As we can see from Figure 4, for any initial configuration, the method converges rapidly to a local maximal. The small oscillation near the end of the simulation comes from numerical discretization error and different mesh generation.

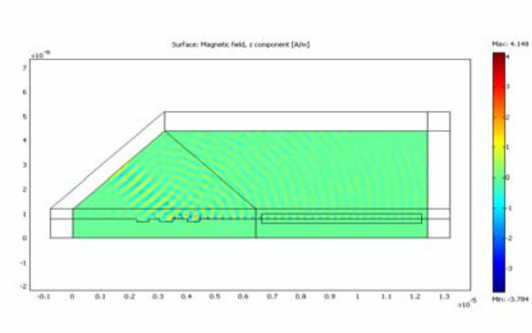

Figure 3. The final optimal design for three gratings

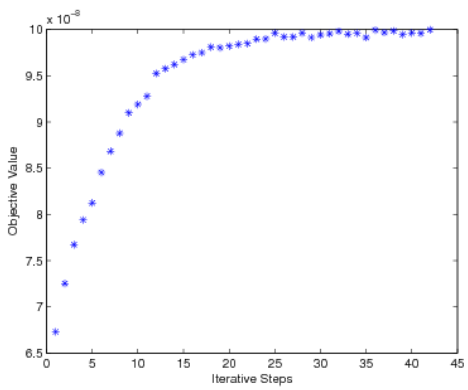

Figure 4. The convergence of the optimization methods

5. Conclusion

An optimal design of the gratings to couple maximum amount of free space photon into surface plasmon wave is implemented by using COMSOL Multiphysics. The optimization procedure is much better than those traditional ones, because the gradients can be calculated much more accurately. Using a gradient ascent approach, the method converges fast to a local optimal design.

6. References

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7. Appendix

Table 1: Parameters used in the simulation

Parameter Name	Symbol	Numerical value
Input Free space light wavelength	$\lambda_0 = 2\pi/k_0$	420 nm
Relative dielectric constant of Ag	ε_m	-4.5365
Relative dielectric constant of SiO_2	ε_d	2.25