Numerical Optimization Technique for the Optimal Design of the Surface Plasmon Grating Coupler

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Abstract: The optimal design of the grating coupler for surface plasmon generation is revisited for its interdisciplinary importance in the efficient use of energy, and the strong dependence of the efficiency of the system on the design. This work contributes a comprehensive gradient based numerical optimization technique and tools to optimize both geometry of the grating and parameters of the Gaussian beam simultaneously. We conduct gradient based optimization in COMSOL-Multiphysics/MATLAB® to obtain a numerical gradient and update the design. The method modifies all geometrical boundaries of each groove independently. The gradient of the objective function is calculated from post processing sensitivity analysis data, and used to update the geometry of each groove in a fixed mesh. Gaussian beam parameters are also optimized simultaneously in the final design. An optimal design shows different groove width, depth, and distance between adjacent grooves. Results obtained show the practical value of these tools to design an efficient n-grooves grating.

Keywords: Finite Element Method, sensitivity analysis, gradient, numerical optimization.

1. Introduction

In quest for the design and development of smaller and more powerful devices, the ability to efficiently use energy is of central importance. Therefore the optimal design of the Plasmon Coupler is of great interdisciplinary interest for its value in enhancing/scattering electromagnetic energy. An efficient plasmon generator is thus an important contribution for practitioners to be able to build better and useful devices.

Excitation of surface plasmons via photons of a light beam directed to a grating-like interface between metal and dielectic produces an enhanced electromagnetic field in a vicinity of this interface. Efficient resonance coupling drives the collective oscillation of the beam of light and charge density on the grating surface of the metal from an input wave to a plasmonic mode with less energy loss. The plasmonic mode excited in this way or SPP has shown great sensitivity to changes in geometry, and characteristics of the incident wave.

Gradient based optimization applied to the optimal design of the grating coupler has produced significant improvement in energy conversion [1][2]. We present a computational tool developed using COMSOL-Multiphysics/ MATLAB® that modifies simultaneously all boundaries of each groove in a silver grating and the design parameters of the input Gaussian Beam in a fixed mesh.

A simple grating coupler for the generation of SPP's is illustrated in Figure (1), with input Gaussian beam.

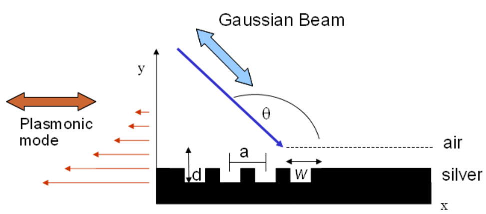

Figure 1: Surface plasmon grating coupler

The grating consists of n-grooves on a silver slab. The size of these grooves {d,w}, separating distance {a} and the parameters of the Gaussian beam such as {θ} are modified during optimization to produce a design that improves the energy conversion.

1.1 Governing Equations

Maxwell Equations govern electromagnetic phenomena. Under simplifying assumptions and the constitutive equations for linear, isotropic, homogeneous media, we obtain Maxwell equations in the frequency domain. This renders a Helmholtz Equation (PDE) in the transverse magnetic H_z for the (x,y) plane:

$$-\frac{\partial}{\partial x}\left(\frac{1}{\epsilon_r}\frac{\partial H_z}{\partial x}\right) - -\frac{\partial}{\partial y}\left(\frac{1}{\epsilon_r}\frac{\partial H_z}{\partial y}\right) = \left(\frac{2\pi}{\lambda}\right)^2 \mu_r H_z. \quad (1)$$

An output coupler design excites a plasmonic mode in the leftmost boundary according to the following equation obtained from [3].

$$H_z(y) = \begin{cases} A_1 e^{-k_2 y} & y \geq 0 \\ A_2 e^{k_1 y} & y < 0 \end{cases}$$
$$k_2 = \sqrt{\beta^2 - k_0^2}, \qquad (2)$$
$$\beta = k_0 \sqrt{\frac{\epsilon_2}{1+\epsilon_2}}$$
$$k_0 = 2\pi/\lambda, \;\; k_1 = -k_2 \epsilon_2,$$

where β is the propagation constant, and $\boldsymbol{\epsilon_2} =$ permittivity of silver at fixed wavelength $\boldsymbol{\lambda} =$ 800 nm.

2. Mathematical Formulation and Model

The optimal design problem after discretization of the PDE by the Finite Element Method (FEM) is:

$$\begin{array}{ll} \max_v & P(J(u,v)) \\ \text{subject to} & Ku = b \\ & g(v) \leq 0 \end{array} \qquad (3)$$

where $P(J) = |J|^2 = (J^r)^2 + (J^i)^2$ is the objective function, u the magnetic field or phasor, v the design parameters, and $Ku = b$ the FEM linear system. J is the complex valued wave coupler functional defined by

$$J = \frac{1}{4} \int_\Gamma \langle (\overline{E}_G \times H) + (E \times \overline{H}_G) \rangle \cdot \vec{n} \, ds, \qquad (4)$$

where, $\{E_G, H_G\}$ are the electric and magnetic field of the Gaussian beam, and $\{E,H\}$ the corresponding FEM approximations in the ouput coupler induced by the plasmonic mode.

The Gaussian beam formula is given by

$$H_G(x,y) = H_0 \sqrt{\frac{w_0}{w}} \exp\left(-\frac{v^2}{w^2}\right) \exp(C) \qquad (5)$$

where

$$C = \left(-jk\left(u + \frac{v^2}{2R}\right) + \frac{j}{2} \arctan\left(\frac{u}{x_r}\right) \right),$$

$u = (x - x_0)\cos(\theta) + (y - y_0)\sin(\theta)$,
$v = -(x - x_0)\sin(\theta) + (y - y_0)\cos(\theta)$,
$x_0 = (x + s) + dist * \cos(\theta)$,
$y_0 = dist * \sin(\theta)$.

in axis of propagation u, radial distance v and the typical Gaussian beam parameters.

The Gaussian beam design parameters are the distances $\{s, dist\}$ and the angle of propagation $\{\theta\}$. The values for $\{s, dist\}$ correspond to the distance from the first groove of the grating $\{x\}$, and the distance from the silver slab to the center of the Gaussian beam respectively. In order to satisfy the size constraint of typical optical fiber the constraint is introduced $dist \geq$ (62.5 e-6m) $\cot(\theta)$. This is illustrated in Figure 2.

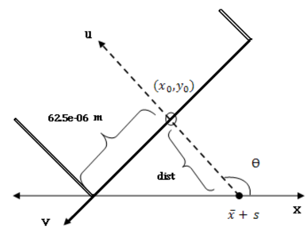

Figure 2: Gaussian beam parameters

The geometric parameters are given for a discrete step at each boundary of a groove denoted as displacement of right (dxR), left (dxL) and bottom (dyB) boundaries. This is illustrated in Figure 3.

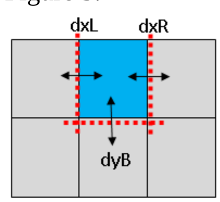

Figure 3: Geometric design parameters

The standard mathematical treatment of separating imaginary and real components is used in this work. The derivative of $P(J)$ is obtained for geometric and Gaussian beam parameters with general form of the derivative of the objective function is:

$$D_v P = 2 J^r D_v J^r + 2 J^i D_v J^i, \qquad (6)$$

In (4) note that the Gaussian beam parameters only modify $\{E_G, H_G\}$, and the geometric parameters affect $\{E,H\}$ exclusively. This separates the formulation of the gradient into two independent parameter sets: analytical Gaussian beam parameters, and numerical geometric parameters. Gradients are then computed using direct differentiation for the geometric parameters in the FEM linear system, and analytical derivatives obtained for the Gaussian beam parameters. Thus the data used to solve the linear system $Ku=b$ is used efficiently to obtain the sensitivity of u to all geometric parameters. The derivatives of P with respect to a geometric parameter v are given by**:**

$$
\begin{aligned}
\frac{\partial J^r}{\partial \mathbf{v}} &= -0.25 \int_{\Gamma} E_G^r \frac{\partial H^r}{\partial \mathbf{v}} + E_G^i \frac{\partial H^i}{\partial \mathbf{v}} \\
&\qquad + \frac{\partial E_x^r}{\partial \mathbf{v}} H_G^r + \frac{\partial E_x^i}{\partial \mathbf{v}} H_G^i \, ds \\
\frac{\partial J^i}{\partial \mathbf{v}} &= -0.25 \int_{\Gamma} E_G^r \frac{\partial H^i}{\partial \mathbf{v}} - E_G^i \frac{\partial H^r}{\partial \mathbf{v}} \\
&\qquad - \frac{\partial E_x^r}{\partial \mathbf{v}} H_G^i + \frac{\partial E_x^i}{\partial \mathbf{v}} H_G^r \, ds.
\end{aligned}
\tag{7}
$$

3. Numerical Optimization Methods

An optimal design is obtained using a numerical gradient by the efficient use of the available solution data from COMSOL-Multiphysics and derived formulas programmed in MATLAB. A gradient of P(J) for geometric parameters is obtained numerically using COMSOL's TM-mode from RF module, the Parameterized Geometry from the Moving Mesh mode (ALE) and the Forward Sensitivity from the Optimization and Sensitivity Analysis module. The analytically obtained formulas for the Gaussian beam parameters of the gradient are coded and the corresponding domains and boundaries updated using MATLAB and applied to the design of the grating coupler**.**

In the TM-mode the PDE in equation (1) with absorbing boundary conditions (ABC) and perfectly matched layer domains (PML) complete the boundary value problem. Figure 4 illustrates the computational domain and boundary conditions. A 4-grooves grating is chosen to modify the geometry by displacement of all boundaries of each groove as seen in Figure 3. The numerical gradient of P(J) with respect to the geometric parameters is obtained from direct differentiation of the FEM linear system $Ku=b$. The forward sensitivity mode uses the solver data for K efficiently. The sensitivity of the state variables u to 11 displacement parameters is obtained in this manner (3 per groove minus a fixed dxL for the first groove).

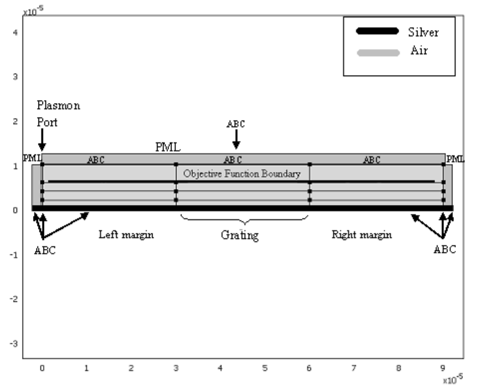

Figure 4: Computational Domain

To compute the sensitivity to the geometric parameters a Parameterized Geometry of the ALE moving mesh mode is defined. The width of a groove can be modified according to the gradient by moving the dxR and dxL boundaries to the left, right or no displacement. Similarly the dyB changes the depth of the groove by displacement upward, downward or no change. The forward sensitivity in the Optimization and Sensitivity Analysis module then computes efficiently the sensitivity of the magnetic field u to changes in the geometry of the grating defined in this way.

The sensitivity of P(J) to the geometric parameters is computed by post processing the forward sensitivity data at the boundary 8e-6 m from the interface according to the obtained formulas. The three Gaussian beam parameters s, $dist$ and θ only require an update of the constants, and therefore can be efficiently obtained from the current solution. This fortunately does not require another solver iteration. In total a 14 dimensional gradient is computed per each solver step.

A fixed mesh is used by defining domains as silver/air according to the permittivity data at λ=800nm. This is accomplished using discrete step updates to increase or decrease the size of each individual groove of the grating.

The algorithm modifies the Gaussian beam parameter as the geometry of the grating changes. When the geometry parameter cannot improve the objective function, the Gaussian beam optimization continues to find the optimal distances {*s*, *dist*} and angle for the best obtained geometry.

4. Results

The Gaussian beam parameter optimization of P(*J*) is conducted on a fixed geometry to obtain the graph in Figure 5.

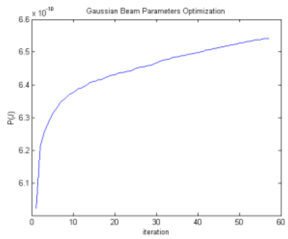

Figure 5: Gaussian beam parameter optimization

A geometric parameter optimization step shows a directional augmentation of the real magnetic field illustrated in Figure 6.

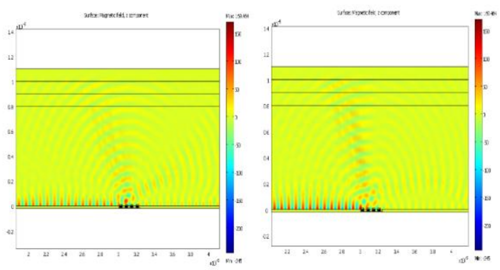

Figure 6: Geometric parameters optimization

The optimal design for the 4-groove grating is illustrated in Figure 7. It confirms that the size of the grooves in the grating is non-uniform. Figure 8 shows the visualization of the real magnetic field of the optimal design.

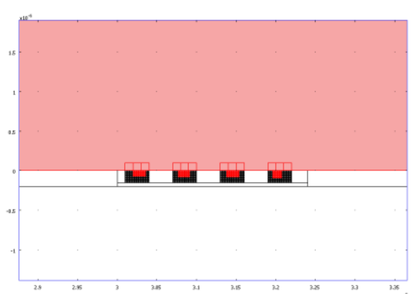

Figure 7: Optimal 4-grooves grating

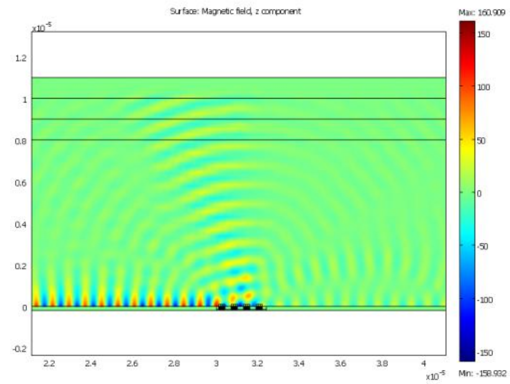

Figure 8: Optimal design Real(H_z)

The conversion rate of the grating improves more than 4 fold as optimal designs are generated. Table 1 summarizes the best designs.

Table 1: Geometry and Gaussian beam 4-groove designs

Design (width X depth) nm	**Gaussian Beam Parameters**	**P e-10**
(100 X 50, 100 X 50, 100 X 50, 100 X 50)	s=5.4e-7m, θ=1.81, dist=1.58e-5m	1.7 (6.3%)
(130 X 80, 120 X 80, 100 X 80, 100 X 80)	s=3.3e-7nm, θ=1.813, dist=1.556e-5m	6.76 (25%)
(160 X 70, 150 X 80, 160 X 80, 120 X 90)	s=3.4e-7m, θ=1.81, dist=1.52e-5m	7.3 (27%)

5. Conclusion

The results show that a non-uniform grating allows significant improvement of the efficiency of surface plasmon generation. The developed tools are suited to modify the geometry of each groove independently and find the optimal Gaussian beam parameters for the modified geometry of the grating that optimizes energy conversion.

The efficient use of solution data obtained from one solver iteration is a strong benefit of this technique. The optimal design tool obtains a 14-dimensional numerical gradient from one FEM solver iteration. This is a promising alternative to a 14 parameter sweep that requires multiple solver calls for each parameter.

The developed tools are of considerable practical value. The optimal design tools can improve a near optimal initial design and provide valuable insight to practitioners on the best design of this nanoplasmonic system.

6. References

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