Optical Spectrum and Electromagnetic-Field Distribution at Double-Groove Metallic Surface Gratings

L. David Wellems¹, D. H. Huang¹, T. A. Leskova², and A. A. Maradudin²

¹Air Force Research Laboratory, Space Vehicles Directorate
Kirtland Air Force Base, NM 87117, USA
²Department of Physics and Astronomy and Institute for Surface Science
University of California, Irvine, CA 92697, USA

Abstract—The Greens function model [8] for calculating the reflection and transmission of light at etched single-groove gratings on both sides of a thin silver film was extended to study the case of double-groove gratings. A splitting of surface-plasmon-polariton (SPP) modes was found due to electromagnetic (EM) coupling between the two grooves in the complex unit-cell of the grating. Spectral features corresponding to the split SPP branches as well as the minigap between them were found in this system. From the full spatial distributions of the total EM field, the high-surface-field regions, the coupling between two grooves in the same complex unit-cell and the coupling between two nearby grooves located at the upper and lower surfaces of the metal film can be identified.

1. INTRODUCTION
Surface plasmons in conductive materials with sub-wavelength structures are a rather interesting research subject, which emerged and attracted attention in recent years [1]. The extraordinarily high transmission of $p$-polarized light propagating through a two-dimensional periodic array of holes with subwavelength diameters, first reported by Ebbeson et al. [2–4], depends strongly on the lattice constant and metal-film thickness in the deep sub-wavelength regime [5]. For a thin metal film on a dielectric substrate, if both the upper and lower surfaces of the film are etched into a linear grating with aligned grooves on both surfaces, the coupling between the two surface-plasmon-polariton (SPP) modes localized at the two surfaces can be spatially modulated due to the variation of the film thickness [6, 7]. Meanwhile, the SPP mode for a planar surface becomes folded with a finite lattice constant and is split into many branches with a minigap either at the center or at the edge of the first Brillouin zone [8]. If a simple unit-cell (SUC) containing only a single groove is replaced by a double-groove complex unit-cell (CUC), each SPP branch will be further split into two branches with a new minigap controlled by an electromagnetic coupling [9] between the two grooves in the CUC. In the case of the CUC with different groove widths and filled dielectric materials, the circulation and weaving of light was found as a result of the excitation of phase resonance [10].

In this paper, we extend the previous spectral calculations [8] for a single-groove grating to include a comparison between results for single- and double-groove gratings. Both the transmissivity and reflectivity spectra are calculated for $p$ polarization. Some new spectral features are found with a double-groove grating, and can be explained by the spatial distribution of the total EM field at these wavelengths.

The paper is organized as follows. In Section 2, we extend the previous model and formalism to include a double-groove grating. The conclusions drawn from these calculations are briefly summarized in Section 3.

2. MODEL AND THEORY
In order to make this paper stand alone, we repeat some of the key steps in deriving the spatial distribution of the EM field as well as the far-field transmissivity and reflectivity. Details of these derivations can be found in the paper by Baumeier, et al. [8].

The scattering system considered in this paper is divided into three regions in the $z$ direction. The region-I for $z ≥ \xi_1(x)$ is for air with a dielectric constant $\epsilon_a$. The region-II for $-h + \xi_2(x) ≤ z ≤ \xi_1(x)$ is filled with a thin metal film with a thickness $h$ and a frequency-dependent complex dielectric function $\epsilon_f(\omega)$ to include the loss effect, where $h\omega$ is the incident photon energy. The
region-III for $z \leq -h + \xi_2(x)$ corresponds to a substrate with a dielectric constant $\epsilon_s$. Here, $\xi_1(x)$ and $\xi_2(x)$ are the profile functions for the patterned upper and lower surfaces of the metal film. In this paper, we will consider only the case of $p$-polarized incident light.

By using Green’s second integral identity \[11\] in the $xz$-plane along with the boundary conditions, we get the following integral Equation \(8\) for the magnetic field $\mathcal{H}_y^{(I)}(x, z)$ within region-I for $z \geq \xi_1(x)$

$$\mathcal{H}_y^{(I)}(x, z) = \mathcal{H}_y^{(\text{inc})}(x, z) + \frac{1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_1} G_a(x, z|x', z') \right]_{z'=\xi_1(x')} \times \mathcal{H}_y^{(I)}(x', z') \bigg|_{z'=\xi_1(x')}$$

$$- G_a(x, z|x', z') \bigg|_{z'=\xi_1(x')} \frac{\partial}{\partial N_1} \mathcal{H}_y^{(I)}(x', z') \bigg|_{z'=\xi_1(x')} \right], \tag{1}$$

where $\mathcal{H}_y^{(\text{inc})}(x, z) = \exp(ikx - i\beta z)$ (with $k = (\omega/c)\sqrt{\epsilon_0} \theta_0$, $\beta = (\omega/c)\sqrt{\epsilon_0} \cos \theta_0$, where $\theta_0$ is the angle of incidence) represents the incident magnetic-field component in $p$ polarization. In a similar way, we can also obtain the integral Equation \(8\) for the magnetic field $\mathcal{H}_y^{(III)}(x, z)$ within region-III for $z \leq -h + \xi_2(x)$

$$\mathcal{H}_y^{(III)}(x, z) = -\frac{1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_2} G_s(x, z|x', z') \right]_{z'=\xi_2(x')} \times \mathcal{H}_y^{(III)}(x', z') \bigg|_{z'=\xi_2(x')}$$

$$- \frac{\epsilon_s}{\epsilon_f(\omega)} G_s(x, z|x', z') \bigg|_{z'=\xi_2(x')} \frac{\partial}{\partial N_2} \mathcal{H}_y^{(III)}(x', z') \bigg|_{z'=\xi_2(x')} \right]. \tag{2}$$

Finally, we obtain the integral Equation \(8\) for the magnetic field $\mathcal{H}_y^{(II)}(x, z)$ within region-II for $z \leq -h + \xi_2(x)$

$$\mathcal{H}_y^{(II)}(x, z) = -\frac{1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_2} G_s(x, z|x', z') \right]_{z'=\xi_2(x')} \times \mathcal{H}_y^{(II)}(x', z') \bigg|_{z'=\xi_2(x')}$$

$$- \frac{\epsilon_s}{\epsilon_f(\omega)} G_s(x, z|x', z') \bigg|_{z'=\xi_2(x')} \frac{\partial}{\partial N_2} \mathcal{H}_y^{(II)}(x', z') \bigg|_{z'=\xi_2(x')} \right]. \tag{3}$$

In Equations \(1\)--\(3\), we have defined

$$\frac{\partial}{\partial N_{1,2}} = -\frac{d\xi_{1,2}(x')}{dx'} \frac{\partial}{\partial x'} + \frac{\partial}{\partial z'}. \tag{4}$$

In addition, the Green’s functions in regions-I(a), region-II(f), and region-III(s) are respectively given by

$$G_{a,f,s}(x, z|x', z') = i\pi Z_0^{(1)} \left[ n_{a,f,s} \left( \frac{\epsilon}{c} \right) \sqrt{(x - x')^2 + (z - z')^2} \right], \tag{5}$$

where $n_{a,s} = \sqrt{\epsilon_0 a_0}, n_f(\omega) = \sqrt{\epsilon_f(\omega)}$ with $\text{Re}[n_f(\omega)] > 0$ and $\text{Im}[n_f(\omega)] > 0$. Moreover, $Z_0^{(1)}(\tilde{w})$ in Equation \(5\) is the zeroth-order Hankel function of the first-kind with a complex argument $\tilde{w}$.

The boundary conditions require both $\mathcal{H}_y^{(I)}(x, z)$ and $(1/\epsilon) \mathbf{n}_0 \cdot \nabla_{xz} \mathcal{H}_y(x, z)$ be continuous across the upper and lower surfaces at $z = \xi_1(x)$ and $z = \xi_2(x)$, where $\mathbf{n}_0$ represents the unit vector along the normal direction of a surface-profile curve and $\nabla_{xz} = (\partial/\partial x, 0, \partial/\partial z)$. Therefore, we obtain the following four equations from Equations \(1\)--\(3\)

$$\mathcal{H}_y^{(I)}(x, z)|_{z=\xi_1(x)} = \mathcal{H}_y^{(\text{inc})}(x, z)|_{z=\xi_1(x)} + \frac{1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_1} G_a(x, z|x', z') \right]_{z'=\xi_1(x')} \times \mathcal{H}_y^{(I)}(x', z') |_{z'=\xi_1(x')}$$

$$- G_a(x, z|x', z') |_{z'=\xi_1(x')} \frac{\partial}{\partial N_1} \mathcal{H}_y^{(I)}(x', z') |_{z'=\xi_1(x')} \right], \tag{6}$$

where
0 = \frac{-1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_1} G_f \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \times H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} - \frac{\epsilon_f(\omega)}{\epsilon_a} G_f \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \frac{\partial}{\partial N_1} H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} \right] \\
+ \frac{1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_2} G_f \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \times H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} \right] \\
+ \frac{\epsilon_s}{\epsilon_f(\omega)} G_f \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \frac{\partial}{\partial N_2} H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} \right] , \quad (7)

H_{y}^{(1)} \left( x, z \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} = \frac{-1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_1} G_s \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \times H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} \right] \\
+ \frac{\epsilon_s}{\epsilon_f(\omega)} G_s \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \frac{\partial}{\partial N_2} H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} \right] , \quad (8)

0 = \frac{-1}{4\pi} \int_{-\infty}^{\infty} dx' \left[ \frac{\partial}{\partial N_2} G_s \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \times H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} \right] \\
+ \frac{\epsilon_s}{\epsilon_f(\omega)} G_s \left( x, z | x', z' \right) \bigg| _{z=\xi_1(x), z'=\xi_1(x')} \frac{\partial}{\partial N_2} H_{y}^{(1)} \left( x', z' \right) \bigg| _{z'=\xi_1(x')} \right] . \quad (9)

To simplify the notation, we denote the four unknowns in Equations (6)–(9) as

S_{\text{(1)}}^{(x)}(x) \equiv H_{y}^{(1)} \left( x, z \right) \bigg| _{z=\xi_1(x)}, \quad (10)

S_{\text{(2)}}^{(x)}(x) \equiv H_{y}^{(1)} \left( x, z \right) \bigg| _{z=-h+\xi_2(x)}, \quad (11)

L_{\text{(1)}}^{(x)}(x) \equiv \frac{\partial}{\partial N_1} H_{y}^{(1)} \left( x, z \right) \bigg| _{z=\xi_1(x)}, \quad (12)

L_{\text{(2)}}^{(x)}(x) \equiv \frac{\partial}{\partial N_2} H_{y}^{(1)} \left( x, z \right) \bigg| _{z=-h+\xi_2(x)} \cdot \quad (13)

Since G_a(x, z|x', z'), G_f(x, z|x', z'), and G_s(x, z|x', z') are all known analytically, Equations (6)–(9) constitute a set of self-consistent nonlocal equations with respect to S_{\text{(1)}}^{(x)}(x), S_{\text{(2)}}^{(x)}(x), L_{\text{(1)}}^{(x)}(x) and L_{\text{(2)}}^{(x)}(x), which can be solved by transforming them into a matrix Equation (8) in a finite range of x. Once the sources S_{\text{(1)}}^{(x)}(x), S_{\text{(2)}}^{(x)}(x), L_{\text{(1)}}^{(x)}(x) and L_{\text{(2)}}^{(x)}(x) in Equations (6)–(9) have been obtained, we can substitute them into Equations (1)–(3) to find the full spatial distribution of H_{y}(x, z) in all three regions including air, metal film and substrate.

Moreover, we can calculate the differential reflection coefficient [8] through the ratio of time-averaged fluxes of energy vertically crossing a xy-plane above z = \xi_1(x)

\frac{\partial R(\theta_s|\theta_0)}{\partial \theta_s} = \frac{cn_a}{8\pi \omega L} \frac{|r(\theta_s|\theta_0)|^2}{\cos \theta_0}, \quad (14)

where \theta_s is the scattering angle, L is the sample length in the x direction, and

r(\theta_s|\theta_0) = \int_{-\infty}^{\infty} dx \exp \left\{ -\frac{i\omega n_a}{c} \left[ x \sin \theta_s + \xi_1(x) \cos \theta_s \right] \right\} \times \left\{ \frac{i\omega n_a}{c} \left[ \frac{d\xi_1(x)}{dx} \sin \theta_s - \cos \theta_s \right] S_{\text{(1)}}^{(x)}(x) - L_{\text{(1)}}^{(x)}(x) \right\} . \quad (15)
In a similar way, we can calculate the differential transmission coefficient [8] through the ratio of time-averaged fluxes of energy vertically crossing a xy-plane below \( z = -h + \xi_2(x) \)

\[
\frac{\partial T(\theta_1|\theta_0)}{\partial \theta_1} = \frac{cn_a |t(\theta_1|\theta_0)|^2}{8\pi \omega L \cos \theta_0},
\]

(16)

where \( \theta_1 \) is the transmission angle and

\[
t(\theta_1|\theta_0) = \int_{-\infty}^{\infty} dx \exp \left\{ \frac{-i\omega n_s}{c} \left[ x \sin \theta_t - \xi_2(x) \cos \theta_t \right] \right\}
\times \left\{ \frac{i\omega n_s}{c} \left[ \frac{d\xi_2(x)}{dx} \sin \theta_t + \cos \theta_t \right] S^{(2)}(x) - \frac{\epsilon_s}{\epsilon_f(\omega)} L^{(2)}(x) \right\}. \]

(17)

By using Equations (14) and (16), we can calculate the reflectivity \( R(\lambda) \) [the transmissivity \( T(\lambda) \)] for normal incidence \( \theta_0 = 0 \) by integrating \( \theta_s (\theta_t) \) over a small interval around \( \theta_s = 0 \) \( (\theta_t = 0) \) in a symmetrical way [8].

For a double-groove grating, we assume the following surface profiles

\[
\xi_1(x) = -d_1 \sum_{j=-\infty}^{\infty} \exp \left\{ -\frac{(x - jb)^2}{a^2} \right\} - d_2 \sum_{j=-\infty}^{\infty} \exp \left\{ -\frac{(x - jb - s)^2}{a^2} \right\} = -\xi_2(x),
\]

(18)

where \( d_1 \) and \( d_2 \) are the depths for two Gaussian grooves, \( b \) is the period of the grating, \( a \) is the decay constant for the Gaussian groove, and \( s < b/2 \) is the separation between the two grooves in the CUC.

In our numerical calculations, we choose silver for the metal material, \( \theta_0 = 0 \), \( h = 110 \text{ nm} \), \( d_1 = 0.4b \), \( b = 600 \text{ nm} \), \( a = 0.1b \) (for a sharper groove), \( L = 400 \lambda \), \( \epsilon_a = 1 \), \( \epsilon_s = 2.1025 \), and \( \epsilon_f(\omega) \) for silver is numerically input from the paper by Johnson and Christy [12].

3. CONCLUSION

By generalizing the Green’s function formalism for a single-groove grating to one for a double-groove grating, we have found the splitting of a surface-plasmon-polariton mode into one symmetrical and one anti-symmetrical mode due to electromagnetic coupling between the two grooves in the same complex unit-cell. Additional peaks in the transmissivity can be found in this system as spectral features corresponding to the split surface-plasmon-polariton branches at individual surfaces of the metal film, which can be identified by the spatial distribution of the total electromagnetic field. From our studies, we have concluded that the split anti-symmetrical surface-plasmon-polariton mode due to the direct electromagnetic coupling in the same complex unit-cell, as well as the cross electromagnetic coupling in different complex unit-cells at both surfaces of the metal film, contribute new spectral features in the transmissivity.

ACKNOWLEDGMENT

Two of authors (TAL and AAM) would like to thank AFRL contract FA 9453-08-C-0230 for partial support. D. W. and D. H. would like to thank the Air Force Office of Scientific Research (AFOSR) for its support.

REFERENCES