Numerical solution for scattering of multilayer noble metal circular aperture arrays nanostructure

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Abstract. Due to its unique properties, metal-dielectric plasmonic structures have been widely applied in many fields, such as light absorption enhancement, surface enhanced spectrum, biosensor, and solar cell. We presented a numerical solution for light scattering from multilayer noble metal circular aperture arrays nanostructure. Using the generalized boundary conditions of surface impedance, the boundary value problem can be transformed into a set of integral equations about current density and magnetic density. Then utilizing the method of moments to solve these integral equations, more accurate reflected, transmitted, and absorbed power expressions can be obtained.

1. Introduction

Since surface plasmon (SP) was presented by Ritchie’s group [1], many scholars have been attracted by its novel optical properties. Surface plasmons is essentially the coupling resonance between the incident photon and the electron near the interface of metal medium. When the frequencies of the two are close or the same, a coupled resonance will occur, resulting in strong light scattering and absorption, or enhancement of local electromagnetic field. Numerous studies have indicated that surface plasmons has broad application prospects in sub wavelength optics, data storage, microscopy, solar cells, and so on. For the past few years, with the development of science and technology, construction, manipulating and observation on the nanoscale have become possible. In particular, Ebbesen found that the extraordinary optical transmission can be achieved through a two-dimensional array of sub-wavelength aperture in thin metal films [2]. The application research of optical nanostructures [3-6], especially the characterization and application of the optical properties of metal nanostructures, has once again aroused people’s attention to the emerging field of plasmon. Due to the unique optical properties, plasmonic metal nanostructures have significant applications in a wide range of areas such as surface-enhanced Raman scattering spectrum [7-9], surface-enhanced fluorescence spectroscopy [10, 11], solar cell [12], biosensor [13, 14] and light absorption enhancement [15]. The results show that the resonance frequency of SP, especially for nanoparticles with tip structure, mainly depends on the morphology of the nanostructure, the geometric size and the dielectric environment.

A numerical solution method is proposed to solve the light scattering field of free-standing multilayer noble metal circular aperture arrays. Using the generalized boundary conditions of the surface impedance, the boundary value problem is transformed into a set of integral equations about current density and magnetic current density. Combined with the expansion coefficient of the current density, utilizing the method of moments to solve these integral equations, more accurate reflected, transmitted, and absorbed power expressions are obtained. Then, from the angle of grating resonance,
the influence of the incident wavelength, various parameters of the metal circular aperture arrays, especially the thickness on reflected, transmitted, and absorbed power are analysed and discussed.

2. Theory and derivation

As shown in Figure 1(a), in \(xy\) plane, a thin noble-metal sheet of thickness \(b\) is perforated with circular apertures arranged periodically, the radius is \(a\), and the period both in \(x\) and \(y\) direction is \(d\).

![Figure 1](image)

And as shown in Figure 1(b), the noble metal film drilled with aperture arrays are stacked in the \(z\) direction with a period \(c\), \(z = z_l = (l - 1)c\) \((l = 1, 2, ..., L)\). It is surrounded by air, with electric constants \(\varepsilon_0\) and \(\mu_0\). As shown in Figure 1(c), a plane wave is incident with a polar angle \(\theta^i\) and an azimuth angle \(\phi^i\). Then we define the wave vector, propagation constants and wave impedance as follow:

\[
\begin{align*}
\mathbf{k}^i &= i_x a_0 + i_y b_0 + i_z c_0 \\
\alpha_0 &= \kappa_0 \sin \theta^i \cos \phi^i, \quad \beta_0 = \kappa_0 \sin \theta^i \sin \phi^i, \quad \gamma_0 = \kappa_0 \cos \theta^i \\
\kappa_0 &= \omega \sqrt{\varepsilon_0 \mu_0} = 2\pi / \lambda, \quad \xi_0 = \sqrt{\mu_0 / \varepsilon_0}
\end{align*}
\]

(1)

where, \(i_x, i_y, \text{and} i_z\) are unit vectors, \(\lambda\) is wavelength. Considering the periodicity of the structure, we only calculate one unit cell in the range of \(|x| < d/2\) and \(|y| < d/2\).

The total electromagnetic field is decomposed as \(\mathbf{E}, \mathbf{H} = (\mathbf{E}^p, \mathbf{H}^p) + (\mathbf{E}^s, \mathbf{H}^s)\), the superscript \(p\) refers to the primary field, and \(s\) refers to the scattered field. If the metal is very thin, far less than the wavelength, and \(|\varepsilon_r| \gg 1\), the generalized boundary conditions [16] on surface \(z = \pm 0\) can be simplified as

\[
\begin{align*}
\frac{1}{2} \left[ \mathbf{E}_T(x, y, +0) + \mathbf{E}_T(x, y, -0) \right] &= R \mathbf{i}_z \times \left[ \mathbf{H}_T(x, y, +0) - \mathbf{H}_T(x, y, -0) \right] \\
\frac{1}{2} \left[ \mathbf{H}_T(x, y, +0) + \mathbf{H}_T(x, y, -0) \right] &= -Q \mathbf{i}_z \times \left[ \mathbf{E}_T(x, y, +0) - \mathbf{E}_T(x, y, -0) \right]
\end{align*}
\]

(2)

where the subscript \(T\) represents the transverse field component. The left side of the equations describe the mean value of the tangential field on both sides of the material, on the right are the electric and magnetic current densities. The proportional constants, which are the electric resistance and magnetic conductance, are expressed as

\[
R = \left( \frac{\xi_0}{l_2 \sqrt{\varepsilon_r}} \right) \cot \left( \frac{\kappa_0 b \sqrt{\varepsilon_r}}{2} \right), \quad Q = \left( \frac{\sqrt{\varepsilon_r}}{i 2 \xi_0} \right) \cot \left( \frac{\kappa_0 b \sqrt{\varepsilon_r}}{2} \right)
\]

(3)

For perfect conductors, there are \(R = 0\) and \(|Q| \to \infty\).

The plane waves of incident, transmission and reflection can be written as
the continuity of the total electromagnetic field on the surface are transformed into the functions of surface current density and magnetic current density. In view of as and in the form of superposition of the Floquet modes as [17-23], the scattered field can be expressed where 

\[
\Psi_1(x,y) - \Psi_2(x,y) = \frac{1}{2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \left( A_{1pq} e^{-i\gamma_{pq} (z-z_l)} + B_{1pq} e^{i\gamma_{pq} (z-z_l)} \right) e^{-i\left( \alpha_p x + \beta_q y \right)} \frac{\sin \left( \frac{\alpha_p x + \beta_q y}{2} \right)}{\sin \left( \frac{\alpha_p x + \beta_q y}{2} \right) k} \sqrt{\alpha_p^2 + \beta_q^2} d
\]

and

\[
\Psi_{2pq}(x,y) = \frac{\alpha_p}{\alpha_p^2 + \beta_q^2} \Psi_{1pq}(x,y)
\]

where

\[
\begin{align*}
\Psi_{1pq}(x,y) & = \beta_q I_x - \alpha_p I_y \\
\Psi_{2pq}(x,y) & = \alpha_p I_x + \beta_q I_y \\
\Psi_{pq}(x,y) & = (\alpha_p^2 + \beta_q^2) I_x / k \sqrt{\alpha_p^2 + \beta_q^2} d
\end{align*}
\]

The constants \( A_{2pq} \) and \( B_{2pq} \) are unknown reflectance and transmission coefficient of the \( pq \)-th mode, respectively. Utilizing the periodicity condition \( \Psi(x + pd, y + qd) = \Psi(x,y) e^{-i(p\alpha_0 + q\beta_0)d} \), and the orthonormal property

\[
\int_{-d/2}^{d/2} \int_{-d/2}^{d/2} \Psi_{pq}(x,y) \Psi_{pq}^*(x,y) dx dy = \delta_{ss} \delta_{pp} \delta_{qq}
\]

where \( \delta_{ss} \) is Kronecker’s delta, the asterisk denotes complex conjugate. Then the unknown functions are transformed into the functions of surface current density and magnetic current density. In view of the continuity of the total electromagnetic field on the surface \( z = \pm 0 \), there are

\[
\begin{align*}
J(x,y) & = \frac{1}{2} l_z \times [H_T(x,y,+,0) + H_T(x,y,-0)] \\
M(x,y) & = -\frac{1}{2} l_z \times [E_T(x,y,+,0) + E_T(x,y,-0)]
\end{align*}
\]

where \( \delta_{ss} \) is Kronecker’s delta, the asterisk denotes complex conjugate. Then the unknown functions are transformed into the functions of surface current density and magnetic current density. In view of the continuity of the total electromagnetic field on the surface \( z = \pm 0 \), there are

\[
J(x,y) = M(x,y) = 0, \quad (|x| < d/2, |y| < d/2, \sqrt{x^2 + y^2} < a)
\]
Combined with the orthogonal equation (9), the modal coefficients of the integral form can be expressed as

\[
\begin{align*}
(A_{1pq}) & = \iint_{\sqrt{x^2+y^2}<a} \left[ \frac{-1}{1+2R\eta_{1pq}} M(x,y) \cdot \Psi^*_{2pq}(x,y) + \frac{1}{2Q + \eta_{1pq}} f(x,y) \cdot \Psi^*_{1pq}(x,y) \right] dx \, dy \\
(B_{2pq}) & = \iint_{\sqrt{x^2+y^2}<a} \left[ \frac{-1}{1+2R\eta_{1pq}} M(x,y) \cdot \Psi^*_{1pq}(x,y) + \frac{1}{2Q + \eta_{2pq}} f(x,y) \cdot \Psi^*_{2pq}(x,y) \right] dx \, dy 
\end{align*}
\]  

and the set of integral equations

\[
\begin{align*}
& \sum_{s=1}^{2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \frac{1}{\zeta_0 \eta_{spq} + 2R/\zeta_0} \Psi_{spq}(x,y) \iint_{\sqrt{x^2+y^2}<a} M(x,y) \cdot \Psi^*_{spq}(x',y') \, dx \, dy \\
& = \frac{\eta_{100} V_1}{\zeta_0 \eta_{200} + 2R/\zeta_0} \Psi_{200}(x,y) + \frac{\eta_{200} V_2}{\zeta_0 \eta_{100} + 2R/\zeta_0} \Psi_{100}(x,y) \\
& \sum_{s=1}^{2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \frac{1}{\eta_{spq} + 2Q} \Psi_{spq}(x,y) \iint_{\sqrt{x^2+y^2}<a} J(x,y) \cdot \Psi^*_{spq}(x',y') \, dx \, dy \\
& = -\frac{\eta_{100} V_1}{\eta_{100} + 2Q} \Psi_{100}(x,y) - \frac{\eta_{200} V_2}{\eta_{200} + 2Q} \Psi_{200}(x,y) 
\end{align*}
\]

where we have used

\[
\eta_{1pq} = \frac{1}{\zeta_0^2 \eta_{2pq}}, \quad \eta_{2pq} = \frac{1}{\zeta_0^2 \eta_{1pq}}
\]

The method of moments [24] is adopted, and solve the integral equations (13) numerically. Normalizing the power by the incident power, then more accurate reflected, transmitted, and absorbed power expressions are obtained as

\[
\begin{align*}
\bar{P}^r_{spq} &= \frac{\zeta_0}{V_0^2 \cos \theta_i} \sum_{s=1}^{2} \eta_{spq} |\bar{B}_{spq}|^2 \\
\bar{P}^t_{spq} &= \frac{\zeta_0}{V_0^2 \cos \theta_i} \sum_{s=1}^{2} \eta_{spq} |\bar{A}_{spq}|^2 \\
\bar{P}^a &= \frac{\zeta_0}{V_0^2 \cos \theta_i} \text{Re} \left[ \sum_{s=1}^{2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \left( |\eta_{spq}(\bar{A}_{spq} + \bar{B}_{spq})|^2 + Q|\bar{A}_{spq} + \bar{B}_{spq}|^2 \right) \right]
\end{align*}
\]

where

\[
\bar{B}_{spq} = B_{spq} + B_s \delta_{p0} \delta_{q0}, \quad \bar{A}_{spq} = A_{spq} + A_s \delta_{p0} \delta_{q0}
\]

3. Numerical results

For simplicity, we only calculated a single silver film with apertures, the radius of aperture \( a \) is 600nm, the period \( d \) is 800nm. A plane wave which the wavelength is from 400nm to 800nm is incident on the aperture arrays perpendicularly. Here, we mainly study the relationship between the scattering field and wavelength of silver films of different thicknesses. The relationship between the reflected, transmitted and absorbed power and wavelength when the thickness of silver sheet is 10nm, 16nm, 20nm, and 30nm is discussed respectively.
Figure 2. Normalized values of total reflected power as a function of wavelength $\lambda$ for different thickness $b$. The size is given by $d = 800$ nm, $a = 600$ nm.

Figure 2 shows the variation of the reflected power corresponding to the incident wavelength when the plane wave is perpendicularly incident on the silver aperture arrays of different thicknesses. It can be clearly seen that, corresponding to the wavelength range from 400 nm to 700 nm, the reflected power increases as the thickness $b$ of the silver film increases, and is proportional to the wavelength (except for the arrays structure with a thickness of 10 nm), and reaches the maximum near 700 nm, while the reflected power of the arrays with a thickness of 10 nm is in a trough. Corresponding to the wavelength range from 700 nm to 800 nm, except for the reflected power of the arrays with the thickness of 10 nm, which shows a sinusoidal change trend, the other reflected power all decrease as the increase of wavelength and thickness.

![Reflected Power vs Wavelength](image1)

Figure 3. Normalized values of transmitted power as a function of wavelength $\lambda$ for different thickness $b$. The size is given by $d = 800$ nm, $a = 600$ nm.

As shown as in Figure 3, except for the arrays structure with a thickness of 10 nm, when the wavelength is less than 700 nm, the transmitted power decreases as the thickness $b$ of the silver film and the wavelength increases, and reaches the minimum near 700 nm. In the range of 700 nm to 800 nm, the transmitted power increase as the decrease of wavelength and thickness. While the transmitted power of the arrays with thickness of 10 nm decreases as the wavelength increases.

In Figure 4, we find that the peak of absorbed power appears at the wavelength closed to 700 nm. Corresponding to the wavelength range from 700 nm to 800 nm, the absorbed power decrease as the thickness of the silver film becomes larger, except for the arrays with thickness of 10 nm. Obviously, when the thickness of the film is less than a certain value, the relationship between the power and wavelength will change.

![Transmitted Power vs Wavelength](image2)

![Absorbed Power vs Wavelength](image3)
4. Conclusion
In this paper, a new numerical analysis method for power distribution is proposed to analyze the light scattering of multilayer noble metal circular aperture arrays nanostructure. The boundary value problem is transformed into a set of integral equations about the electric and magnetic current density, and solved by the method of moments. The results show that, when the appropriate aperture parameters and the incident wavelength are selected, the transmission power can be significantly increased, and the reflection power can also be reduced. Similarly, the appropriate parameters can be selected to significantly enhance the absorbed power. Obviously, by using this analytical method, a more accurate expression of the scattered field can be obtained. This is of potential value for further research on the influence of metal nanostructure parameters on the scattering field, designing reasonable optical devices to improve the absorption of photovoltaic devices, and to reduce the geometric thickness of photovoltaic absorbing layer of solar cells.

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