Collective behavior of impedance matched plasmonic nanocavities

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Abstract: Nanometer sized cavities arranged as a subwavelength metallic grating can provide omni-directional and complete absorption of light. We present an explanation of this extraordinary phenomenon as a collective resonant response of a system based on a surface impedance model. This model gives a straightforward way to design systems for optimum light trapping performance and as well gives fundamental insights into the interaction of light with metals at the nanoscale.

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References and links


1. Introduction

The design and fabrication of plasmonic structures for light trapping is a highly active area of research with a wide range of applications ranging from solar energy conversion to field enhancement for non-linear optics [1,2]. Many of these systems are constructed from an ensemble of identical units in a subwavelength grating structure. When considering light coupling to such structures, a fundamental question becomes whether these units can be treated independently or must be treated in terms of a collective excitation of the system. A structure for complete light trapping and strong field enhancement has been proposed by Le Perchec et al. [3] (illustrated in Fig. 1), where the phenomenon was explained on the basis of the action of a single 5-nm-wide nano-groove (NG) where the excitation of coupled surface plasmons polaritons (SPP) on the walls of the groove led to the system behaving as an interference Fabry-Perot nano-cavity. We have recently realized a practical demonstration of this effect [4]. The same assumption that the performance of these types of systems can be modeled on the basis of a single unit has also been followed in a number of other studies [5–8]. However, it is well known that collective effects can play an important role in determining the behavior of some types of plasmonic systems [9–14]. We connect the analysis of a single resonant NG narrower then the metal skin depth to the collective excitation of the subwavelength grating and present a simple relationship between the NG width $w$, height $h$, and period $p$ required to achieve omni-directional and complete light absorption at the metal surface.

2. Intergroove interaction

To give an insight into the fundamental nature of this phenomenon, we have developed a surface impedance-based analytical model for complete omni-directional light absorption in the NGs and present its comparison to Finite Difference Time Domain numerical calculations. We

![Fig. 1. Schematic of the plasmonic nano-grooves on a metal surface. The SPPs propagate down the NG along the z-axis, then reflect off the bottom and travel back to the mouth. On resonance, all incident energy is trapped within the grooves.](image-url)
Fig. 2. Reflectivity response for a combined double grating where one NG set is inserted in between another one. The dimensions for the sets NG1 and NG2 are $w_1 = 19$ nm, $h_1 = 45$ nm, $w_2 = 10.8$ nm, and $h_2 = 56.1$ nm. Period for both gratings is $p = 300$ nm. The independent behavior of the two gratings when combined shows that, on resonance, the SPPs traveling on the flat surface do not contribute to the reflectivity response of the NG grating.

begin by examining the general features of the light-SPP interaction to define the region of validity for an analytical theory. When light interacts with a sharp metal edge, as in case of a grating structure, SPPs are generated along the top surface as well as inside the grooves (for an experimental time resolved study of this effect see the work by Kubo et al. [15]). To determine which SPPs contribute to the on-resonance absorption, we first consider two gratings NG1 and NG2 optimized for complete absorption at different wavelengths. These give the reflectivity responses as shown by the dashed lines in Fig. 2. When two such gratings are interleaved, a composite structure is formed with the unit cell as shown in the inset of Fig. 2. The design of this system is such that the SPPs generated by NG1 that travel on the top surface are blocked by NG2, yet the reflectivity response of the composite grating is a linear combination of the reflectivity responses of NG1 and NG2 (see the solid curve in Fig. 2) similar to the independent transmission of the photon sorters [16]. This independent behavior of each grating, when put in combination, shows that on-resonance, the top-surface SPPs do not contribute to the reflectivity response of the subwavelength grating.

However, in a dense grating the neighboring NGs can interact via the evanescent fields of the SPPs travelling down the walls of the NGs. Figure 3 illustrates the reflectivity effect of this interaction for small (a) and large (b) grating period, where reflectivity is plotted for $\lambda_0 = 800$ nm normal incidence light when $w$ is held constant and $h$ is varied from 0 to 1.5 $\mu$m. From the set of reflectivity dips the SPP wavelength inside the groove can be calculated using the Fabry-Perot analysis: $2k_{pl}h_m + \phi = 2\pi m$, where $k_{pl} = k'_{pl} + ik''_{pl} = \frac{2\pi}{\lambda_{pl}}$ is the plasmon wave vector, $m$
Fig. 3. Effect of the NG period on the reflectivity response in gold. The NGs constitute a set of resonant cavities: (a) SPP field penetration into the metal is the dominant factor for a dense grating, where complete absorption is achieved only for extreme \( h \); (b) in a sparse grating NGs act as resonant cavities useful for field enhancement and field localization close to the metal surface. The inset shows the change in the real part of the plasmon wavelength due to the change in the NG period.
is the index of each dip and \( h_m \) is the corresponding depth. In this way, the dispersion relation is numerically calculated for a given NG width and varying NG period; the result is shown in the inset of Fig. 3(b). The plasmon wavelength varies from the incident light wavelength (for \( p \) close to \( w \)) to the SPP dispersion in the metal-insulator-metal (MIM) waveguide [17] as \( p \) approaches the wavelength of light \( \lambda_0 \). For a 10 nm wide NGs in gold, the SPP evanescent wave decay length in the metal is given by [18] \( 1/|\sqrt{\varepsilon_{metal}}[2\pi/\lambda_0]^2 - |k_{pl,z}|^2| \approx 30 \) nm. The overlap between the evanescent fields from the neighboring NGs can be neglected for \( p > 100 \) nm, but is significant for \( p = 50 \) nm. For such a dense grating achieving complete absorption requires micron-deep NG channels due to the long SPP wavelength. The case of interest, where the reflectivity extinction occurs for \( h < 70 \) nm yielding strong field enhancement [6] and field localization close to the metal surface, is shown in Fig. 3(b) corresponding to a sparse grating. The distance corresponding to the overlap of the evanescent fields sets the lower limit on the region of validity for the analytical model presented here.

As the period is further increased, for wavelengths of light close to the NG period, the SPPs generated at the metal surface in between the NGs can outcouple to photons due to the addition of the grating momentum. To quantify this effect, we have defined angular bandwidth as the angle of incidence where reflectivity reaches 0.5 starting from 0 at normal incidence (Fig. 4 shows reflectivity calculated for a range of angles of incidence). Achieving complete absorption for NG periods approaching the wavelength of light yields extremely narrow angular bandwidth and the reflectivity response becomes that of a regular grating: a sharp resonance that is highly angle dependent. Therefore, the upper limit on the region of validity for the analytical model is approximately the wavelength of light \( \lambda_0 \).

Achieving the resonance condition requires a set of NG period, width, and height, which, in the range of validity \( w << p < \lambda_0 \), can always be found by numerical optimization to produce on-resonance reflectivity consistently below 0.1%. For the following discussion, the reflectivity is measured when the geometry of individual NGs is optimized to produce such resonance for a given wavelength of light. The resulting NG dimensions are plotted in Fig. 5 along with the characteristic spectral bandwidth (FWHM) of the resulting reflectivity dip (for reflectivity spectrum examples see Fig. 2). In the context of our model a subwavelength grating can be optimized for both large spectral and angular bandwidth yielding omni-directional (see the bottom left inset of Fig. 4) complete light absorption at the metal surface.

3. Theoretical model for the on-resonance behavior
The model for the on-resonance behavior of such subwavelength gratings consists of calculating the surface impedance due to the ensemble of the NGs, each of which are treated as independent radiation sources. This model is valid only for the on-resonance behavior, when \( h \) is set to satisfy the resonance condition for a given pair \((w, p)\). Therefore, quantities like the cavity \( Q \)-factor and the SPP wave vector inside the cavity \( (k_{pl}) \) are expressed as a function of only \( w \) and \( p \).

For \( p \)-polarization, where the E-field of the incoming light is polarized perpendicular to the orientation of the NGs (as shown in Fig. 1) the H-field is approximately constant across the flat surface and the mouth of the NG [3]. From the boundary conditions, the electric field at the metal surface away from the NGs is close to zero, which is equivalent to an out-of-phase sum of the incoming and reflected waves. In this case, the reflected H-field is in phase with the incident H-field, and hence the amplitude is doubled: \( H_{surface} \approx 2H_0 \). It is important to note that no reflected wave exists in the far field, so this approximation is only valid at the metal boundary. On resonance, all the incoming electric field at the metal interface is trapped within the NG [3], and is further amplified due to the NG cavity [6]: \( E_{surface} = E_0 \times Q_w/p \), where \( Q \) is the NG quality factor that will be defined below.

The reflectivity \( R \) can be expressed in terms of the complex reflection amplitude coefficient \( r \)
Fig. 4. Angular bandwidth is affected by the NG period. As the period is increased approaching the wavelength of incident light the angular bandwidth sharply drops and the reflectivity response acquires more of a grating-like character: a sharp resonance that is highly sensitive to the angle of incidence and wavelength.

and the surface impedance [12], which captures the effect of the ensemble of the NGs: $Z_{surf} = \frac{E_{surf}}{H_{surf}}$, where $Z_0$ is the impedance of free space.

$$Z_{surf} = \frac{E_0}{H_0} \times \frac{w \cdot Q}{p \cdot 2}$$  \hspace{1cm} (1)

$$R = rr^*, \hspace{0.3cm} r = \frac{Z_{surf} - Z_0}{Z_{surf} + Z_0}$$  \hspace{1cm} (2)

Substitute the relationship $E_0/H_0 = i \times k_{pl}c/\omega = i \times k_{pl}/k_0^R$ from the solutions to Maxwell’s equations for a transverse magnetic monochromatic plane wave [17] ($H_z = H_x = E_y = 0$), where $k_0^R = \omega/c$ is the on-resonance wave vector of the incident light. The final expression for the surface impedance of an ensemble of the NGs becomes:

$$Z_{surf} = i \times \frac{k_{pl}}{k_0^R} \times \frac{w}{2p} \cdot Q$$  \hspace{1cm} (3)

Next, consider the fields inside the individual grooves. On resonance, the mode in the NG forms a standing wave, where H- and E-fields travel 90° out of phase, and have the same mouth-to-bottom amplitude variation. In this way, the $Q$-factor can be defined as the ratio between the $H$-field at the bottom to $H$-field at the mouth of the NG: $H_{bottom} = Q \times H_{top}$, $H_{NG} = 2H_0 \cos(k_{pl}z)$. On resonance, the plasmon wave vector can be rewritten using $\Delta k_{pl} = k'_{pl} - k_{pl}^R$ to be $k_{pl} = k_R^P + \Delta k_{pl} + ik''_{pl}$, where $k_{pl}^R$ is the SPP wave vector on resonance. Taylor expanding the cosine term yields the final expression for $Q$: 
Fig. 5. Resonant behavior of the nano-groove. Producing a minimum reflectivity on-resonance at constant incident wavelength for a range of NG periods requires adjusting the NG dimensions. In the region of validity (shown in gray background), the analytic model presented here agrees well with the numerical FDTD calculations on the absolute scale as shown in (a). On the relative scale, the NG period-to-width ratio—shown in (b)—is flat in the validity region, which is closely approximated by our model: the NG width increases linearly with the period accompanied by bandwidth (FWHM) narrowing as shown for Au (black) and Cu (blue).
\[ Q = \frac{2}{\pi} \times \frac{1}{\Delta k_{pl} + i \frac{k_{pl}'}{k_{pl}}} \]  

(4)

The \( \Delta k_{pl} \) term can be rewritten in terms of the derivative \( dk_{pl}/d\omega \):

\[ \frac{\Delta k_{pl}}{k_{pl}'} = \frac{dk_{pl}}{k_{pl}'} \frac{\Delta \omega}{\omega} \frac{\omega_R}{\omega} = \frac{\Delta \omega}{\omega} \frac{dk_{pl}}{d\omega} \frac{\omega_R}{k_{pl}'} \]  

(5)

Putting together equation 4 for an individual NG for \( k_{pl} \rightarrow k_{pl}' \) with the effect of an ensemble of NGs given by Eq. (3) yields:

\[ Z_{surf} = i \times \frac{\alpha/\omega}{\Delta \omega/\omega + i \cdot \beta/\omega}, \left\{ \begin{array}{l} \alpha/\omega = \frac{1}{Z_0} \frac{\omega c}{\pi p} \frac{k_{pl}'}{k_{pl}'} \frac{d\omega}{dk_{pl}} \\ \beta/\omega = \frac{1}{\omega} \frac{d\omega}{dk_{pl}} \end{array} \right. \]  

(6)

Equation (2) can now be rewritten in terms of energy lost due to radiation \( \alpha \) and energy dissipation in the metal \( \beta \):

\[ R = \frac{\Delta \omega^2 + (\alpha - \beta)^2}{\Delta \omega^2 + (\alpha + \beta)^2} \]  

(7)

On resonance, when \( \Delta \omega = 0 \), the optimum geometry of the NG yields a balance between the radiative loss and the energy dissipation in the metal: \( \alpha = \beta \). The period-to-width relationship then is given by:

\[ \frac{p}{w} = \frac{1}{\pi} \frac{[k_{pl}']^2}{k_{pl}'' k_{pl}'} \]  

(8)

4. Results and discussion

A case study was performed for copper and gold: a comparison between the analytical model given by Eq. (8) and the FDTD calculations for 800 nm normal incident light is shown in Fig. 5. In the region of validity, the \( p/w \) ratio from the analytical model is in excellent agreement with the FDTD simulation for both materials (see Fig. 5(a)). The small disagreement in the absolute value for the \( p/w \) ratio—as seen in Fig. 5(b)—is attributed to the effects of the SPPs propagating on the surface in between the NGs, which is beyond the present model. This effect is more prominent in the case of gold where the flat surface SPP dispersion relation lies closer to the light line, rendering top-surface SPP coupling more efficient than in the case of copper.

An analogy to an electronic circuit can be made using the idea of surface impedance. For example, for copper, using Eqs. (3) and (4), throughout the region of validity the surface impedance \( Z_{surf}^{Cu} = Z_0 \pm 5\% \). Tuning the NG geometry and period can be understood as an impedance matching phenomenon. Most importantly, for practical applications the subwavelength grating can be designed to be impedance matched for both maximum angular and spectral bandwidth (see Figs. 4 and 5). The period-to-width relationship given by Eq. (8) is a powerful tool in designing subwavelength plasmonic gratings for omni-directional complete light absorption at the metal surface.

5. Conclusions

In summary, the model we have presented leads to a new insight into the collective interaction of plasmonic nanostructures. It also gives a simple and powerful method for optimization of
these structures for practical applications in areas as diverse as solar energy conversion and field concentration for non-linear optics.

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