Light scattering and plasmon resonances in a metal film with sub-wavelength nano-holes

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Abstract. We report on a theoretical study of optical extinction in a metal film of 15-230 nm in thickness patterned periodically with sub-wavelength nano-holes of 140 nm in diameter. The gold plate was on a thick SiO$_2$ wafer and the nano-holes as well as the top side of the metal plate were filled with water or solvent. Light was sent in toward the plate from the SiO$_2$ side. The simulations were performed by solving the Maxwell equations using the scattering matrix method. It was seen that the extinction can, depending on the periodicity of the hole array, show one or several peaks in the visible wavelength range. The positions of the peaks were redshifted when the thickness of the gold plate was decreased. It was found that the peak positions for a thick plate can be identified from a simple surface plasmon dispersion relation.

1. Introduction
The interaction of light with structures having sub-wavelength details can give rise to surprising effects, especially if metals are present. A metal-dielectric interface can support electromagnetic surface modes [1], i.e., surface plasmons (SPs). Incident light can couple to these modes and periodically corrugated metals can lead to both enhanced [2–4] and suppressed [5] transmission of light. In this work we study the (optical) extinction in a gold plate with periodically patterned nano-holes. The dependencies on the thickness of the plate, the periodicity of the nano-hole array, and the refractive indexes of the materials surrounding the plate are considered. Such a gold plate is of experimental interest since it can be used as a bio-sensor when the nano-holes and the top side of the plate is filled with a solvent and the shift of the extinction peak due to a change in the refractive index of the solvent is observed [6].

2. Method
The system is modeled with the classical Maxwell equations. It is assumed that the materials are simple and non-magnetic. The generalised Ohm’s law is assumed to hold. Under these assumptions the only parameter that characterises the system is the generalised permittivity, \( \varepsilon \), which is obtained in this work from tabulated values of the bulk index of refraction, \( n \), through

\[
\varepsilon(x, \omega) = \epsilon_0 n(x, \omega)^2,
\]

where \( \epsilon_0 \) is the permittivity in vacuum and \( \omega \) the frequency of incident light. Light is assumed to propagate in the \( z \) direction and there exists a scattering system, which can be sliced in the \( z \) direction so that \( \varepsilon(x, \omega) \) is \( z \) independent in each slice. Furthermore it is assumed that the system is periodic in the \( x \) and \( y \) directions with periods \( L_x \) and \( L_y \), respectively.
By working with only the $x$ and $y$ components of the fields an eigenvalue equation is obtained for the plane wave expansion coefficients of the fields. The solutions of this eigenvalue equation give forward and backward propagating modes in each slice. With boundary conditions from the Maxwell equations at the interface between two adjacent slices the eigenmode expansions in the two slices can be matched [7]. Finally by introducing the scattering matrix [8], $S$, the fields scattered by the system can be calculated for a given incident light. The introduction of $S$ gives numerical stability since backward propagating modes that could cause numerical overflow are not explicitly present in the calculations.

3. The system
The simulated system consists of a gold plate of thickness $t$ sandwiched between SiO$_2$ on the left and H$_2$O or solvent on the right as shown in Fig. 1. There is a periodic array of holes in the gold plate, see Fig. 2. The holes have diameter $D$ and the periods of the array are $L_x$ and $L_y$ in the $x$ and $y$ directions, respectively. The holes are filled with H$_2$O or solvent. Light is sent in from the left in a direction normal to the plate. Tabulated values are used for the refractive index $n$ of gold [9], H$_2$O [10] and SiO$_2$ [11].

4. Results
We study the (optical) extinction, $\eta$, which is defined as

$$\eta = \log_{10} \frac{I_{\text{inc}}}{I_{\text{tr}}} \quad (2)$$

where $I_{\text{inc}}$ and $I_{\text{tr}}$ are the incident and transmitted light intensities, respectively.

We start by considering a system with $L_x = L_y = 333$ nm and $D=140$ nm. The thickness dependence of the extinction is shown in Fig. 3 for $t = 15 - 230$ nm. It is seen that for the considered thickest plate there is an extinction peak at wavelength $\lambda = 570$ nm. The position of the peak redshifts as the thickness of the plate decreases. If the simulated extinction spectra for the 15-25 nm thick plates are compared to results for an experimental system [6] with the same hole diameter and average hole coverage it is found that the peak positions are in good agreement with the experimental observation. The simulated spectra, however, show much stronger extinction peaks. One reason for this might be that the holes were randomly located in the experiments in contrast to the periodical arrays assumed in the simulations. Furthermore there was a thin Cr layer between the gold plate and the SiO$_2$-wafer in the experiments. Results when the Cr layer is taken into account are shown in Fig. 4 for a 20 nm thick plate. It is seen that the peak is strongly dampened already when a 1 nm thick Cr layer is present.
Figure 3. Extinction spectra for a system with $D = 140$ nm, $L_x = L_y = 333$ nm, and different values of thickness $t$. The curve with highest peak is for $t = 230$ nm and subsequent curves are for $t = 140, 80, 40, 25, 20,$ and $15$ nm.

Figure 4. Extinction spectra for a system with $t = 20$ nm, $D = 140$ nm, and $L_x = L_y = 333$ nm in the presence of a Cr layer of different thicknesses $d$ between the gold plate and the SiO$_2$ wafer. The curve with the highest peak is for $d = 0$ nm and the subsequent curves are for $d = 1, 2, 3$ nm.

A planar interface between two materials with permittivities $\tilde{\varepsilon}_1$ and $\tilde{\varepsilon}_2$ can support SPs if one of them is a metal. The dispersion relation for these SPs is given by [1]

$$k_{sp} = \frac{2\pi}{\varepsilon_0 \lambda} \left( \frac{\tilde{\varepsilon}_1(\lambda)\tilde{\varepsilon}_2(\lambda)}{\tilde{\varepsilon}_1(\lambda) + \tilde{\varepsilon}_2(\lambda)} \right)^{1/2},$$

where $k_{sp}$ is the SP wave vector and $\lambda$ is the wavelength of light in vacuum. Incident light can excite SPs of the same frequency. However, when a planar periodic structure is present in the two-material system, only certain SP modes can be excited. For instance, for a periodic structure with periods $L_x = L_y = L$, the wave vector of the excited SPs satisfies

$$k_{sp} = \frac{2\pi}{L} \sqrt{m^2 + n^2},$$

where $m$ and $n$ are integers, giving the SP mode numbers $(m, n)$. If a metal plate is thick enough it should support two sets of SP modes, one at each interface, where the dispersion relation for each set is given by the single interface dispersion relation in Eq. (3). When a more general dispersion relation for SPs in thin films [1] was considered, it was found that $t = 230$ nm was thick enough for using Eq. (3) as a good approximation for the materials considered in this work.

The extinction spectra for varying $L_x = L_y$ are shown in Fig. 5 for $t = 230$ nm. When these peak positions are compared to the wavelengths of the allowed corresponding SP modes given in Table 1 for the corresponding planar interface with a periodic pattern of periods $L_x = L_y = L$, one can find an excellent agreement. Figure 6 shows the results of the calculations to see how the changes in the refractive index of the materials surrounding the gold plate affect the extinction spectra. Here the study has been made for increases of the refractive index on the SiO$_2$ side and for decreases of it on the solvent side. The periods, $L_x = L_y$, are fixed to 450 nm, and $t = 230$ nm. Comparison of the peak positions in Fig. 6 with the corresponding wavelengths given in Table 2 again shows an excellent agreement.

5. Conclusion
In conclusion, we have studied optical extinction properties of a metal film patterned periodically with sub-wavelength nano-holes. The calculated extinction spectra show a good agreement with
Table 1. Wavelengths, $\lambda^{(\text{interface},(m,n))}$, in nm at which SP modes can occur at an Au-SiO$_2$ or a Au-H$_2$O interface for a planar periodic structure with periods $L_x = L_y = L$. The wavelengths in the range of 520-1010 nm are considered.

| $L$ (nm) | $\lambda^{(\text{H}_2\text{O}/\text{Au})}$ | $\lambda^{(\text{SiO}_2/\text{Au})}_{(1,0)}$ | $\lambda^{(\text{SiO}_2/\text{Au})}_{(1,1)}$ |
|----------|--------------------------|--------------------------|--------------------------|
| 333      | -                        | 570                      | -                        |
| 360      | 555                      | 595                      | -                        |
| 400      | 595                      | 640                      | -                        |
| 450      | 646                      | 700                      | 554                      |

Table 2. Wavelengths, $\lambda_{(m,n)}$, in nm at which SP modes can occur at an interface between Au and a material with refractive index $n$ for a planar periodic structure with periods $L_x = L_y = 450$ nm.

| $n$ | $\lambda_{(1,0)}$ | $\lambda_{(1,1)}$ |
|-----|-------------------|-------------------|
| 1.1 | 547               | -                 |
| 1.2 | 590               | -                 |
| 1.55| 744               | 582               |
| 1.65| 790               | 611               |

Figure 5. Extinction spectra for a system with $t = 230$ nm, $D = 140$ nm, and $L_x = L_y = 333$ nm (dotted line), 360 nm (dashed line), 400 nm (dash-double dotted line) and 450 nm (solid line).

Figure 6. Extinction spectra for a system with $t = 230$ nm, $D = 140$ nm, and $L_x = L_y = 450$ nm. Solid line and dotted line are for the cases when the refractive index on the SiO$_2$ side is increased to $n = 1.65$ and 1.55, while dash-double dotted line and dashed line are for the case when $n$ on the solvent side is decreased to $n = 1.2$ and 1.1.

Experiments and the positions of the extinction peaks for a thick plate are found to coincide with the wavelengths obtained from the simple SP dispersion relation for planar interfaces.

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