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Theoretical analysis of gold nano-strip gap plasmon resonators

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Abstract. Gold gap plasmon resonators consisting of two nm-thin and sub-micron-wide gold strips separated by a nm-thin air or quartz gap are considered. Scattering resonances and resonant fields are related to a model of resonances being due to counter-propagating gap plasmon polaritons forming standing waves. A small gap (~ 10 nm) is found to result in small resonance peaks in scattering spectra but large electric field magnitude enhancement (~ 20), whereas a large gap (~ 100 nm) is found to result in more pronounced scattering peaks but smaller field enhancement. Design curves are presented that allow construction of gap plasmon resonators with any desired resonance wavelength in the range from the visible to the infrared, including telecom wavelengths. The relation between resonance wavelength and resonator width is close to being linear. The field magnitude enhancement mid between the gold strips is systematically investigated versus gap size and wavelength.

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1. Introduction

Metal nano-structures are interesting from an optical point of view because of the possibility of large local electromagnetic fields near such structures when they are illuminated with light, which can be used for sensing and spectroscopy purposes [1]. It has also been argued that metal nano-wires can work as optical antennas being much smaller than the wavelength of the light considered [2, 3], and significant attention has recently been given to the resonant optical behavior of metal rods and wires [4]–[7].

It was recently established for the related geometry of nm-thin and sub-micron-wide gold or silver strips that the main physical explanation for scattering resonances was related to the excitation of counter-propagating slow surface plasmon polaritons (PPs) forming standing wave resonances [8, 9]. In this paper, we will consider a related geometry based on two such gold strips separated by a nm-thin gap in which a similar explanation of scattering resonances worked for silver [10]. Although absorption losses are higher, we have chosen here to consider gold nano-strips instead of silver, since some work has already been done for silver [10], and since gold is a more practical material for experiments because silver oxidizes when exposed to air. We also include the case of quartz as a surrounding material since such a surrounding material is less academic than the case of air, and in that case we have recently demonstrated for single-nano-strip resonators excellent agreement between theory and experimentally measured scattering resonances [11]. Also of usefulness for experiments is the investigation presented of the relation between resonance wavelengths and structure geometry. Recently, a near-linear relation between resonance wavelength and nano-strip width was found for single nano-strip resonators [12, 13] for a wide wavelength range from the visible to the infrared [12].

The case of two closely spaced metal strips considered here does hold some similarity to the cases of a single strip or a square-shaped thin metal plate placed close to a metal surface in which case scattering (or extinction) and local fields have also been considered [14]–[19]. In that case an extra scattering channel is scattering into surface PPs propagating along a single metal interface, which is an important scattering channel for small strip-to-metal-surface separations (<50 nm) [26]. The optical properties have also been investigated for the related geometry of thick metal films separated by a thin gap, where it was shown that light can be squeezed into a 3 nm-thick gap [20, 21].

The paper is organized as follows: in section 2, some basic properties of gap PPs are reviewed. In section 3, it is demonstrated that scattering resonances of gap plasmon resonators

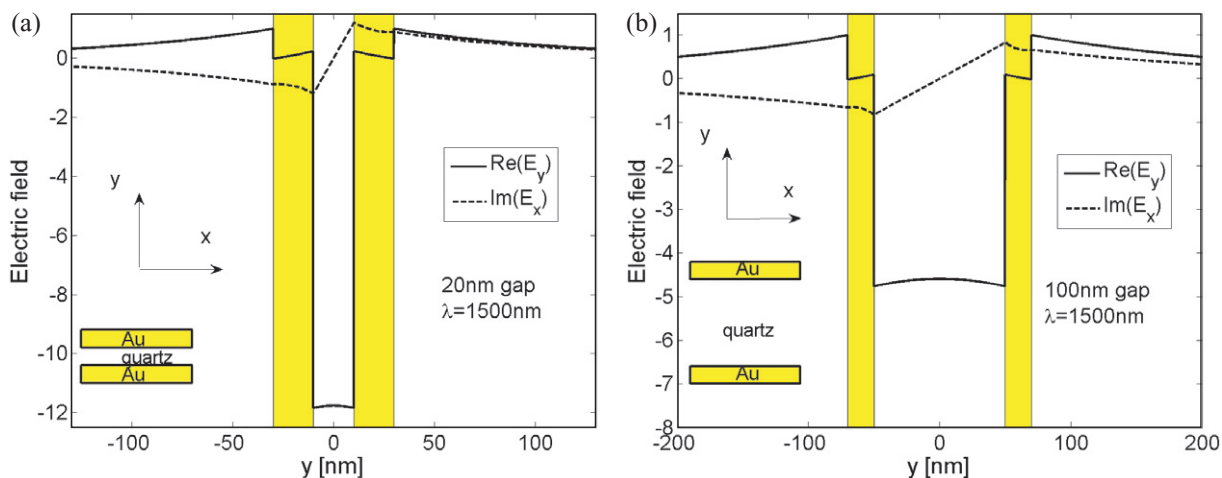


Figure 1. Field distribution for a gap PP in a configuration of two 20 nm-thick gold films separated by (a) 20 nm or (b) 100 nm, and surrounded by quartz.

can be explained in terms of counter-propagating gap PPs forming standing wave resonances. The relation between resonance wavelength and resonator geometry is mapped out in section 4, and local electric field magnitude enhancement is studied in section 5. The conclusion is given in section 6.

2. Gap PPs

Since our physical interpretation of resonances in the resonant structures considered is based on gap PPs, we will briefly sketch their optical properties. Gap plasmons exist in a structure consisting of two gold films of e.g. thickness 20 nm, separated by a narrow gap of 20 nm (figure 1(a)) or 100 nm (figure 1(b)) with quartz in the gap and quartz surrounding the metal films. The gap plasmon is a type of electromagnetic wave that is strongly localized to the gap between the gold films, bound to the system of the two films, and it propagates along the films in their plane. According to the coordinate system in the insets of figure 1 this means that the wave can propagate e.g. along the x -axis and is confined along the y -axis. The electric field vector will be of the form

$$\mathbf{E}(x, y) = \mathbf{E}(y) e^{-i\beta x}, \quad (1)$$

where β is the propagation constant, β/k_0 is known as the mode-index, $k_0 = 2\pi/\lambda$ is the free-space wave number, and λ is the free-space wavelength. Gap plasmons are p-polarized waves, which means in this case that the electric field does not have a z -component. Examples of the field distribution for gap PPs for a 20 and 100 nm gap and the wavelength 1500 nm are presented in figure 1. Note the large field in the gap and the exponential decay of the field along the y -axis away from the system of the two strips. The fields were calculated by a method similar to the one presented in [10] for silver gap plasmon resonators. In this method, the field in each layer is described as two plane waves propagating along the x -direction as $\exp(-i\beta x)$ and along the negative and positive y -axes as $\exp(\pm i\kappa y)$, where $\beta^2 + \kappa^2 = k_0^2 \epsilon$, where β is a constant and ϵ is the dielectric constant of the medium being considered. The waves are, in our case, evanescent along the y -axis. The coefficients of the plane waves on one and the other side of the layered

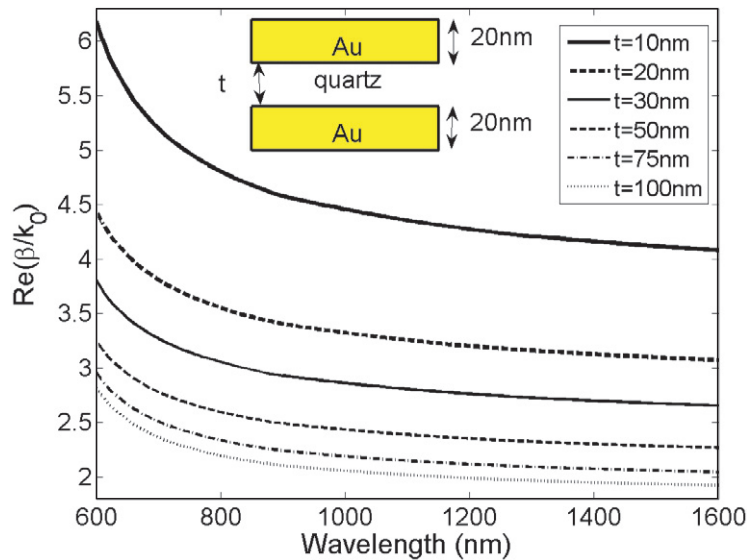


Figure 2. Real part of the mode-index versus wavelength for gap PPs being primarily confined in a gap of thickness t between two gold films of thickness 20 nm. The gold films are surrounded by quartz.

structure are related by a 2×2 matrix, and the requirement that the wave decays exponentially away from the layered structure leads to the requirement that a matrix coefficient must equal zero. Since this coefficient depends on β , this requirement works as a determinant equation that determines the allowed values of β and thereby the mode-index of the bound modes propagating along the x -axis. Throughout the paper, our modeling results are based on the refractive index 1.452 for quartz and the data of Johnson and Christy [22] for gold, with linear wavelength interpolation between available data points. For example, for gold and the wavelengths 800 and 1500 nm, we have used the refractive indices $0.15 - i * 4.90$ and $0.68 - i * 10.34$, respectively.

The gap plasmon polaritons are not the only type of waves supported by the system of two metal films. Other types of waves exist that are more weakly bound and with less strong field in the gap. However, for our purpose, the gap PPs are the most interesting waves, since because of their strong confinement and large mode-index they can be efficiently reflected at structure terminations, whereas more weakly bound waves are reflected less efficiently and are therefore less interesting for making a resonator.

The mode-index of the gap PPs is shown in figure 2. It increases with decreasing gap size t and, at least for the wavelength range considered here, with decreasing wavelength. Note that in all cases considered, the mode-index is significantly higher than the refractive index of the surrounding dielectric material 1.452.

3. Fundamental and higher order resonances in gold gap plasmon resonators

In this section, we will demonstrate the idea that resonances in resonator configurations such as the ones shown in the insets of figures 3 and 4 are due to counter-propagating gap PPs forming standing waves. Compared with the structures considered in section 2, we still consider only propagation in the xy -plane and p-polarized fields. While we assume the structures to

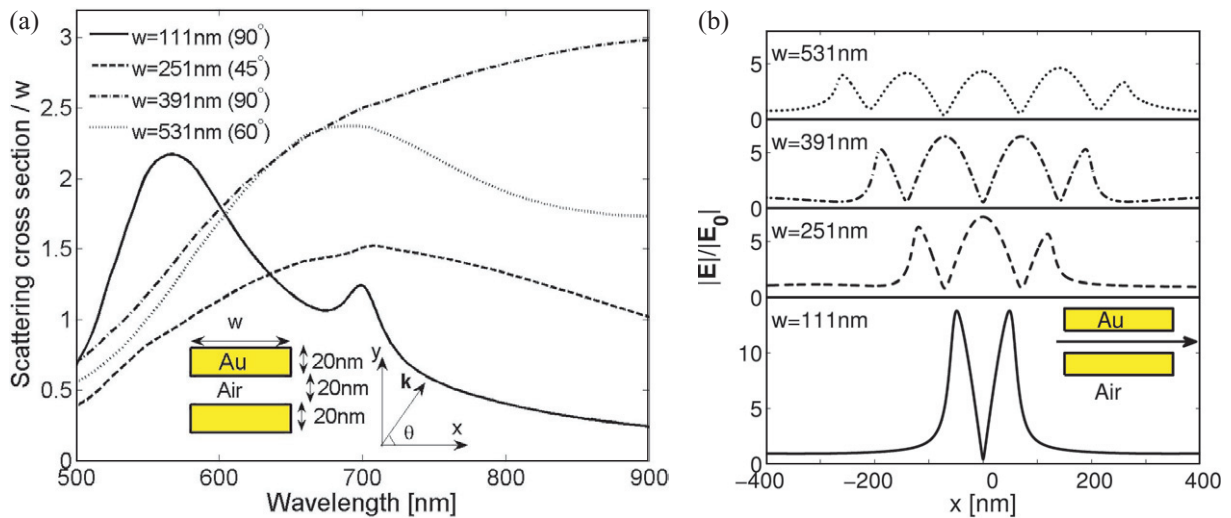


Figure 3. (a) Scattering cross section versus wavelength for a resonator made of two gold (Au) nano-strips surrounded by air being illuminated with a p-polarized plane wave propagating in the direction of the vector \mathbf{k} given by the angle (θ) indicated in the legend. (b) Electric field magnitude relative to the incident light wave (\mathbf{E}_0) along a line through the center of the gap plasmon resonator at the resonant wavelength 700 nm for different strip widths.

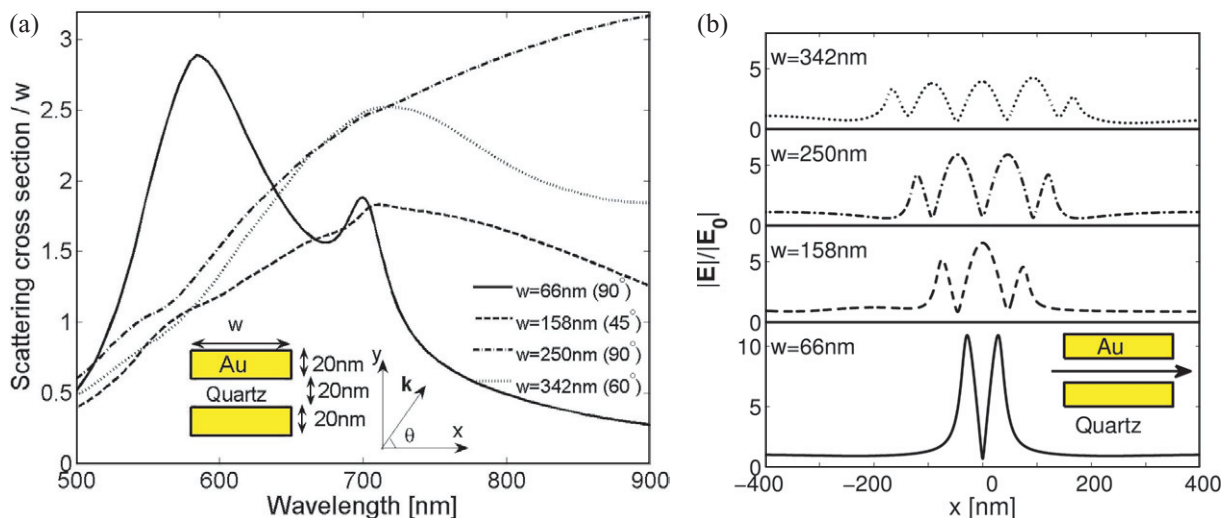


Figure 4. Same situation as figure 3 except that the gold strips here are surrounded by quartz.

be infinite along the z -axis as before, the gold structures are now of finite width along the x -axis. Nevertheless, gap PPs can still propagate along the x -axis over the short sub-wavelength distances considered, and upon reaching the structure termination, the gap PPs can be efficiently reflected into backwards propagating gap PPs, and standing wave resonances can be formed for certain wavelengths. With this Fabry–Perot-like interpretation of resonances, the resonance

wavelength λ must satisfy the following equation:

$$w \frac{2\pi}{\lambda} n_{\text{pp}} \approx m\pi - \phi, \quad (2)$$

where w is the width of the resonator, $n_{\text{pp}} = \text{Re}(\beta/k_0)$ is the real part of the mode-index of the gap PP, ϕ is the phase change related to reflection of PPs at the resonator terminations and m is an integer referring to the order of the resonance. We do not know exactly the reflection phase. However, according to equation (1) we can predict that in the case of a gap plasmon resonator with resonance wavelength λ , another resonator with the same resonance wavelength can be obtained by increasing the width of the resonator by half a gap PP wavelength ($\lambda/2n_{\text{pp}}$). This concept is illustrated in figures 3 and 4 for gold gap plasmon resonators in air and quartz surroundings, respectively. Electric fields and scattering cross sections related to the gap PPs were obtained by the Green's function surface integral equation method (see e.g. [23]–[26]).

In the case of air surroundings (figure 3), we find a scattering resonance at the wavelength $\lambda = 700$ nm for two gold strips of width $w = 111$ nm and thickness 20 nm being separated by a 20 nm air gap. This resonance corresponds to the case $m = 1$ in equation (2). Half a gap plasmon wavelength in this case is equivalent to $\lambda/2n_{\text{spp}} = 140$ nm, and indeed when increasing the resonator width by 140 nm a scattering peak is again found at the wavelength $\lambda = 700$ nm although it is very small. A scattering peak is hardly observable at $\lambda = 700$ nm for the third- and fourth-order resonances. Nevertheless, the field images (figure 3(b)) reveal that for all the resonance orders 1–4 the field through the center of the gap plasmon resonator resembles a standing-wave field pattern matching the resonant order. Thus a resonance is still there even though it is practically not observable in the scattering cross section. The longer propagation distances involved per roundtrip in the case of larger m and correspondingly larger w result in larger propagation losses (per roundtrip), and the main loss mechanism degrading the resonator quality factor is the ohmic losses due to light absorption by the gold. Also note that scattering for different resonance orders was calculated for different propagation directions of the incident p-polarized plane wave. The incident field propagates along the direction given by the angle relative to the x -axis (see figure 3(a)) specified in the legend of the figure. The propagation direction was chosen to optimize the scattering peaks and field strengths (figure 3(b)). For example, the direction 90° cannot be used for exciting second- and fourth-order resonances due to symmetry mismatch between incident field and resonant field. For a similar calculation for silver gap plasmon resonators [10], scattering peaks were also clearly observable for third- and fourth-order resonances. This can be explained by the fact that ohmic losses in silver at the considered wavelength (700 nm) are considerably smaller.

Similar calculations are presented in figure 4 for gap plasmon resonators consisting of gold and quartz. In this case, we notice that the resonator width is significantly smaller, e.g. only $w = 66$ nm for the first-order resonance, which is then comparable with the total height of the resonator of 60 nm. The scattering cross section is larger but the field magnitude at resonance is slightly smaller. A more detailed investigation of the field enhancement will be presented in section 5.

4. Fundamental resonance versus resonator geometry

In this section, we will focus on the fundamental resonance ($m = 1$) and study in detail the relation between the resonance wavelength, the strip width and the gap between the strips.

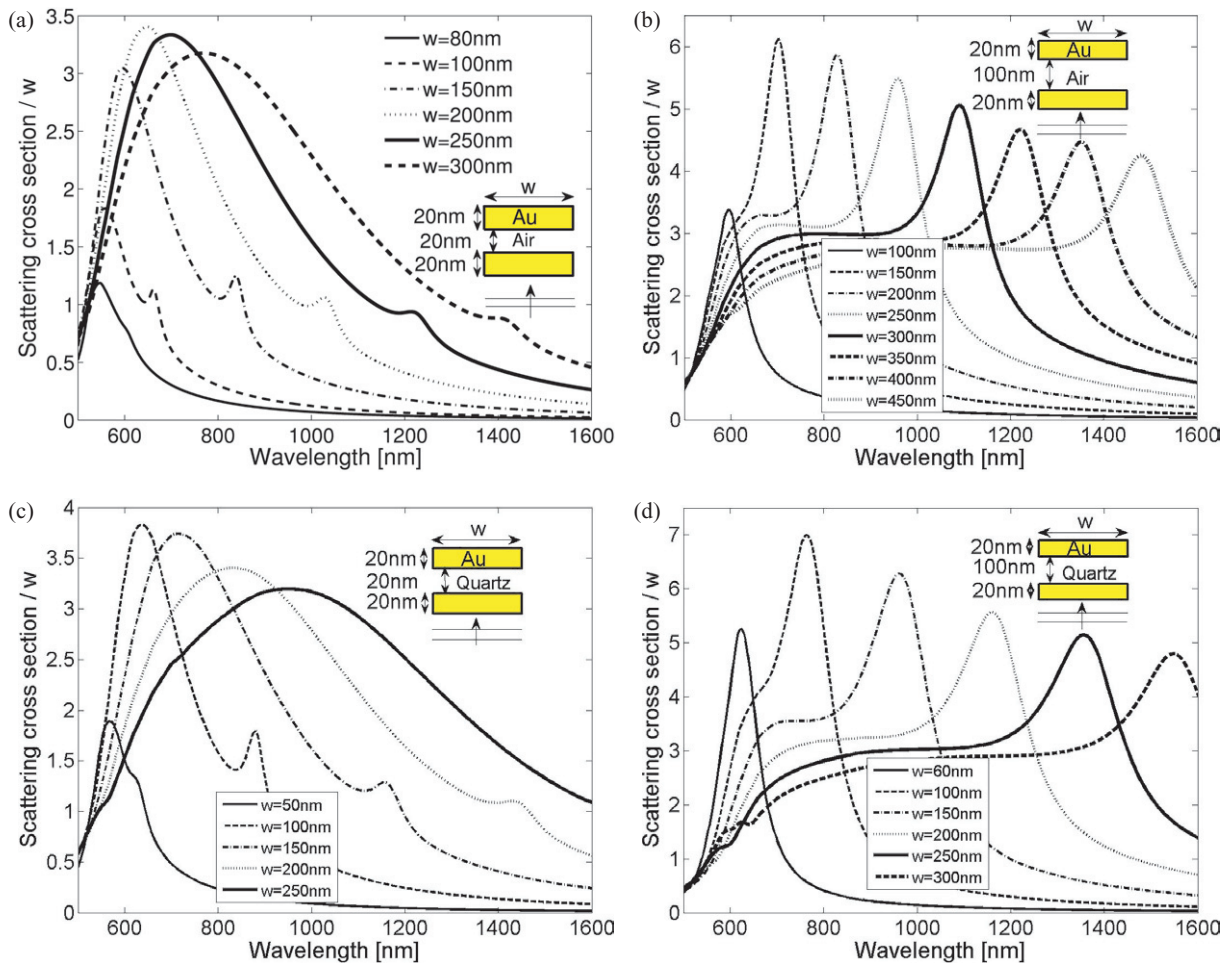


Figure 5. Examples of scattering spectra covering wavelengths from the visible to the infrared for gap plasmon resonators with 20 nm-thick gold strips separated by 20 or 100 nm and surrounded by air or quartz (see insets). The resonators are bottom-illuminated (see inset) with a p-polarized plane wave.

Examples of scattering spectra in the case of bottom-illuminated strips (90° angle of incidence) for varying strip width and gap sizes 20 and 100 nm and for air and quartz surroundings are shown in figure 5 for wavelengths from the visible to the infrared including telecom wavelengths (~ 1500 nm).

The examples of spectra reveal that for small gaps (20 nm) between the gold strips, the scattering resonances are small and in some cases seen only as a shoulder rather than a scattering peak. On the contrary, much more pronounced scattering peaks are found in the case of a large separation (100 nm) between strips, which indicates that the scattering peaks in this situation will be much easier to observe experimentally. The gap plasmon resonator clearly does not work only for optical wavelengths but scattering resonances can also be considered for the infrared and telecom wavelength range.

The fact that the scattering cross section becomes small for wavelengths approaching ~ 500 nm is due to the properties of the dielectric constant of gold. The decrease seen in the scattering spectra for long wavelengths is because there are no further scattering peaks for wavelengths beyond that of the first-order resonance.

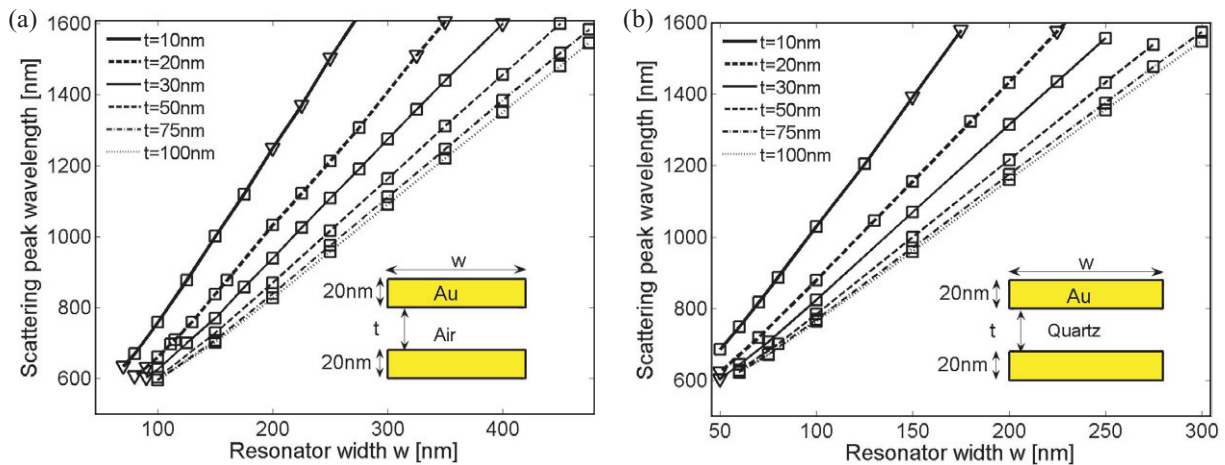


Figure 6. Wavelength of the first-order scattering resonance for gap plasmon resonators consisting of 20 nm-thick gold strips in (a) air, or in (b) quartz, versus strip width w for different distances t between the strips. A square means that the data point was obtained from a scattering peak, whereas an inverted triangle means that the point was estimated from a shoulder in a scattering spectrum.

From scattering calculations such as figure 5, each scattering peak or shoulder can be related to a specific geometry, and it is possible to map out the relation between resonance wavelength, strip width and gap size. Such a map is presented in figure 6 for the air (figure 6(a)) and quartz (figure 6(b)) surroundings.

The near linear relation between the resonator width and scattering resonance wavelength is similar to what was found for strip resonators based on a single strip [12]. Notice that for equation (2) to predict a near linear relation between resonator width and resonance wavelength, the reflection phase must also be wavelength-dependent. From equation (2), we can expect that since the gap PP mode index n_{pp} decreases with increasing gap size t , then the resonance wavelength must also decrease, which is observed in figure 6. Equation (2) also predicts straightforwardly that more wavelength shift is obtained per unit of width change in the case of quartz surroundings compared with air surroundings (figure 6). Also notice that the curve change with increasing t becomes small when t is ‘large’, which is related to small changes in the mode-index with increasing t when t is large (see figure 2). Note that much larger separations than $t = 100$ nm are necessary before the scattering spectrum would resemble that obtained for the case of only one metal strip [10].

5. Field enhancement

For the case of gap plasmon resonators based on 20 nm-thick silver strips separated by 20 nm and surrounded by air, we recently found for the similar situation an electric field magnitude enhancement of ~ 30 mid between the strips from a figure similar to figures 3(b) and 4(b). Here for the same wavelength, the same strip thicknesses and separation, the value found for gold structures is only approximately half as large (figure 3(b)— $w = 111$ nm).

A systematic investigation of the field enhancement mid between gold strips is presented in figure 7. We notice that it is possible to achieve more than a factor ~ 20 in field enhancement

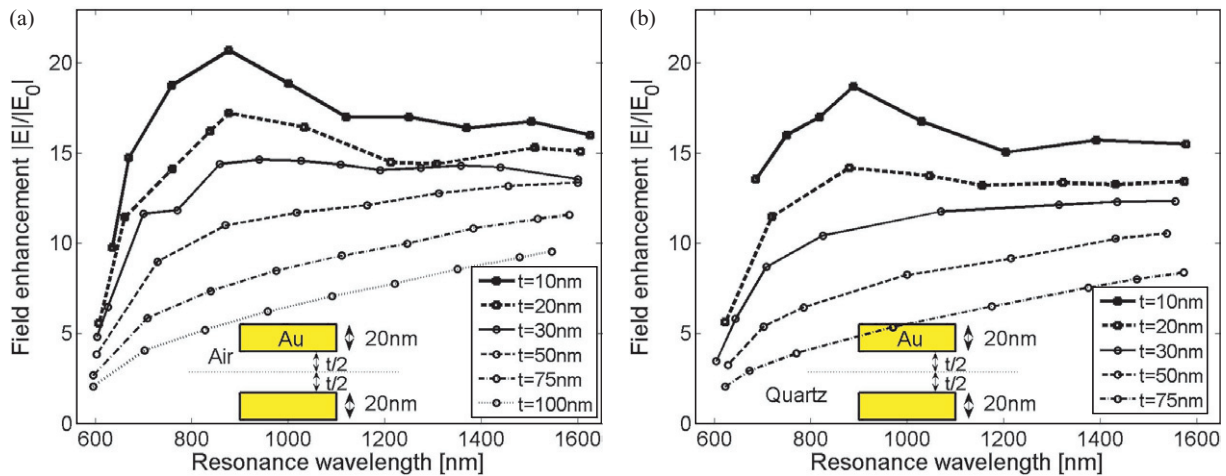


Figure 7. Maximum electric field magnitude enhancement along a line through the center of the gold gap plasmon resonator surrounded by (a) air or (b) quartz.

with the gold gap plasmon resonator by using a 10 nm separation between strips in the case of wavelengths around 900 nm. Longer wavelengths are favorable for gold, since gold and silver then become more similar regarding ohmic losses. A trend observed (figure 7) is that larger field enhancement can be obtained when decreasing the strip separation t . Also, at least for larger separations, the field enhancement increases with increasing wavelength, which in a sense follows the same trend since the gap size t in that case becomes smaller compared with the wavelength. The field enhancement found in the case of quartz surroundings is smaller compared with the case of air. Again, however, in that case the optical distance between the strips is larger, and this is therefore in agreement with the general trend of decreasing enhancement with increasing gap size.

It appears that the largest field enhancement is found for small strip separations when the scattering resonances are the weakest, and that the weakest field enhancement is found when scattering resonance peaks are clearly seen (large gap size t). This can be expected since large scattering means that light couples more efficiently out of the resonator and into propagating waves, which decreases the resonator quality factor and thereby the strength of the resonant field.

6. Conclusion

It was demonstrated for resonators of two 20 nm-thick gold strips separated by a 20 nm gap that scattering resonances were related to counter-propagating gap PPs forming standing waves. By increasing the width of the strips by half a gap PP wavelength, a resonance was found again for the same wavelength (700 nm). A peak in the scattering spectrum was only practically observable for first- and second-order resonances. However, also for third- and fourth-order resonances, field calculations revealed a standing-wave field pattern and thereby standing-wave gap plasmon resonances.

The relation between first-order resonance wavelength, strip width and separation between strips was mapped out for 20 nm-thick gold strips surrounded by quartz or air. The relation between wavelength and strip width was found to be close to linear.

Scattering resonances in the case of a large separation between strips (~ 100 nm) was predicted to be much easier to observe experimentally compared with the case of a small separation (~ 10 – 20 nm), since in the latter case the resonance shows up in scattering spectra only as a very small peak or a shoulder. On the other hand if the main interest in the resonators is due to their ability to enhance the electric field magnitude locally, it will actually be the case of small separation, which is very interesting since a systematic investigation of field enhancement showed a trend of increasing field enhancement with decreasing separation.

Acknowledgments

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