Resonant optical transmission through the sub-wavelength air-hole arrays in a gold thin film for sensing applications

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Abstract. We have investigated numerically the optical spectral properties of resonant transmission of light through sub-wavelength air-holes in a gold thin film by using the finite element method. The enhanced transmission can be comprehended in the light of interfering surface-wave-like modes propagating in the sub-wavelength air-holes. The effects of geometrical and material properties of the sub-wavelength air-holes in the transmission spectrum were characterized. The proposed structure can be operated as refractive index (RI) sensor with a sensitivity of 524.8 nm/RIU (RIU = refractive index unit) ranging from the visible to the near-infrared. This feature provides a remarkable scheme of nanoscale sensing for the RI variations of the environmental media such as applications in liquid and gas sensing.

1. Introduction

Nanostructured metallic films and their transmission properties are potential for both fundamental studies of light-matter interaction and for developing nanophotonic devices based on surface plasmon resonances (SPRs) [1]. Recently, the SPR effect on metal nanoparticles (MNPs) has been followed out in the related fields of nanophotonics [2]. The optical properties of sub-wavelength air-holes in metallic thin films have been investigated extensively because of the discovery of enhanced optical transmission through such a structure [3]. The enhanced transmission in arrays of sub-wavelength air-holes can be realized to be since the surface plasmon polaritons (SPP) propagating on the metal film [4], or the coupling of incident EM wave into sub-wavelength air-holes waveguide modes [5], or the diffraction theory [6]. SPRs have shown great potential for applications in sub-wavelength optics with components such as the sensitivity of SPRs on the surrounding environment has been exploited in various sensors [7] and nanophotonics device applications [8]. The resonances have also been made use of in surface-enhanced spectroscopy [9].

In this paper, the transmission spectrum of x-polarized (transverse magnetic) light through a two-dimensional (2D) periodic sub-wavelength air-holes array in an Au thin film by using three-dimensional (3-D) finite element method (FEM) is investigated and analyzed. The transmission resonance of a single sub-wavelength air-hole as a sensor is proposed to use for detecting small changes in the refractive index (RI) of the surrounding medium. The sensor could be used, for example, to detect biological molecules. By using progressive techniques of nanofabrication [10], the proposed sensor could be integrated in various lab-on-chip applications.
2. Simulation Method And Models
Numerical simulations in this work are performed by using 3-D FEM based on Maxwell's equations. Figure 1 shows the schematic diagram of the truncate view of a 2-D periodic array of air-holes in a gold (Au) thin film with thickness $t$ (Fig. 1 (a)) and its unit cell (Fig. 1 (b)). To imitate an infinite periodic array, the simulation model is obtained from the unit cell by performing a periodic boundary condition (PBC) along both the $x$- and $y$-axes (the lateral directions of the unit cell) and the anisotropic perfectly matched layers (PML) condition on the top and bottom surfaces of the unit cell to diminish the influence of light reflection. A 3-D meshing with a high density tetrahedral mesh is used in the simulation structure and the surrounding matrix. The value of the incident electromagnetic (EM) wave is fixed at $|E_0|=1 \text{V/m}$ to be normally incident from the top surface of the structure. The parameters used in this work are $\Lambda$ (period along the $x$ and $y$ axes), $t$ (thickness of the Au thin film) and $R$ (radius of the circular air-hole in the Au thin film) and the environmental medium is set to be 1.0 for air. The transmittance ($T$) can be obtained from the scattering parameters (S-parameter), i.e., $S_{21}=(\text{power from the reflected light plane})/(\text{power from the incident light plane})^{1/2}$. Transmittance is calculated by $|S_{21}|^2$.

![Figure 1](image_url)

**Figure 1.** Schematic diagram of the simulation model, (a) truncate view of a periodic array of circular air-holes in an Au thin film, and (b) schematic plot of a unit cell of circular air-hole in an Au thin film. The parameters used in the simulations are listed in the inset of this figure.

3. Results And Discussion

3.1. Transmittance spectrum
It is necessary to investigate the transmission spectrum of a periodic air-holes array with different radius ($R$) and period ($\Lambda$) in an Au thin film to demonstrate which transmission peaks correspond to the resonant localized waveguide (RLW) modes [9], and to know their dependencies. Figures 1 (a)-(e) show the calculated transmittance spectrum of different radius ($R=50$, 75, 100, 125 and 150 nm) and period ($\Lambda=400$, 450, 500, 550 and 600 nm) in an Au thin film with a thickness of $t=100$ nm. Several groups of resonance peaks of the transmittance spectrum are observed in Figs. 2(a)-(e). These transmission peaks are the RLW modes and their magnitudes can be tuned by changing their radii and periods. In all transmission spectra, the smaller ones are located at the ultra-violet (UV) wavelengths while the larger ones are in the range of the visible spectral region, which become stronger as $R$ is increased and $\Lambda$ is decreased. The period $\Lambda$ indicates the density of the air-hole arrays in the Au thin film and has a significant contribution to the transmission spectra. The enhanced transmission magnitude with respected to a larger $R$ and a smaller $\Lambda$ can be intuitively understood since more flux of light (i.e., increasing the $R$ and number of holes (i.e., decreasing the $\Lambda$) per unit area (i.e., decreasing the $\Lambda$) lead to more light being transmitted through the air holes. Note that the period $\Lambda$ denotes the density of the air-hole arrays in the Au thin film and has a significant
contribution to the transmittance spectra. It can be demonstrated from Figs. 2 (a)-(e) that the transmittance increases as the value of the period is reduced. This is due to the coupling effect of the shorter period among the air-hole arrays in the Au thin film, as oppose to weaker coupling effect for a longer period. Next, we consider the effect of the thickness of the Au film on the transmittance spectrum. Figure 2(f) depicts the transmittance spectra for different thickness of an Au film ($t=100, 150, 200, 300$ and $400$ nm) with a period $\Lambda$ and a radius $R$ fixed at $400$ nm and $100$ nm. The result indicates that as the $t$ is decreased, the resonance wavelength ($\lambda_{res}$) peaks become significantly higher. Note that the transmittance increases and that the $\lambda_{res}$ peak shifts to the red with decreasing $t$, whereas the transmission spectra become weaker as $t$ is increased. As the RLW becomes shorter (i.e., smaller $t$), the real part of the propagation constant of the RLW mode increases. This corresponds to a higher real part of the effective index of refraction, and thus to a shorter optical length of the cavity in the air-holes, which clarifies the red shift of the $\lambda_{res}$ peak.

Figure 2. (a)-(e) Transmittance spectrum of different radii ($R=50, 75, 100, 125$ and $150$ nm) and period ($\Lambda=400, 450, 500, 550$ and $600$ nm) in the Au thin film with a thickness of $t=100$ nm. (f) Transmittance spectra for different thickness of the Au film ($t=100, 150, 200, 300$ and $400$ nm) with a period $\Lambda$ and a radius $R$ fixed at $400$ nm and $100$ nm.
3.2. Near-field intensity and surface charge distributions

The above analysis could be further identified with the near-field intensity and surface charge distributions of air-holes in the Au thin film with different R and Λ with respect to their corresponding λres (results not shown here). We find that surface plasmons can be excited surrounding their surfaces and rims. The x-component of the electric field (Ex) shows two distinct petals of distribution on the top and bottom sides, showing no electric fields in the air-holes. The y-component of the electric field (Ey) is distributed symmetrically along the rim aperture of the air-holes, showing four crossing petals of distribution. In contrast to Ex, the z-component of the electric field (Ez) shows two distinct petals of distribution on the left and right sides, showing more electric fields in the air-hole. The total field distributions (Etotal) at their corresponding resonances show a hybridized plasmon mode on the metallic rim surfaces and in the air-holes, and the strongest field intensity is found in the central part of the air-holes. Owing to different in the number of free electrons, the induced positive-negative surface charge pairs on the rim aperture of the air-holes enhanced each other by induced electromotive force. This behavior could be interpreted by the fact that the increased number of free electrons along the rim aperture of the air-holes affected not only the magnitude of induced surface current but also the full-charging time on the edge area [10].

3.3. Surface plasmon resonance sensing application

To realize the detailed behavior of the field intensity distribution around the air-holes arrays in the Au thin film under SPR excitations, Fig. 3(a) shows the near field intensity corresponding to resonant wavelength versus different radius of air-holes with R= (50, 75, 100, 125, 150) nm along the x-axis measured at the middle plane of the Au thin film in the range of x= [-200, 200] nm. It is shown that the higher near field intensity can be found at R=75 and 100 nm, while the lower near field intensity occurred at R=50, 125 and 150 nm, respectively. A distinct edge enhancement of the field intensity can be found among the rim aperture of the air-holes. The positive-negative charge pairs on the Au thin film surface can be considered as many dipoles at the symmetry positions around the circumference of the rim aperture air-holes. The x-polarization field intensity pattern can be understood as a strong dipolar excitation that involves the entire ring perimeter. Note that the localized electric field enhancement at the edge along the air-hole is due to the edge enhancement effect [11].

![Figure 3](image.png)

Figure 3. Near field intensity corresponding to resonant wavelength versus different radius of air-hole with R= {50, 75, 100, 125, 150} nm along the x-axis measured at the middle plane of the Au thin film in the range of x= [-200, 200] nm. (b) Transmittance spectra for fixing t=100 nm, Λ=400 nm and R=75 nm as the different material within the air-holes of Au thin film.

In order to verify the dependence of the transmittance resonance on the material surrounding the Au air-hole thin film, the transmittance spectra for air (n = 1.0), water (n = 1.33), glass (n = 1.52), and
optical oil ($n = 1.63$) were investigated (Fig. 3 (b)). The geometrical parameters are fixed at $t=100$ nm, $\Lambda=500$ nm and $R=75$ nm. As the RI of the air-hole medium increases, the $\lambda_{res}$ has a significant red shift. The transmittance peak position made a red-shift with a slight increase in magnitude whenever a fluid of higher RI was introduced into the Au thin film with the air-holes arrays. With the increase of RI, a red-shift of the transmittance peak varied from 610 to 940 nm. The sensitivity ($S=\Delta\lambda/\Delta n$) raised to a value of 523.8 nm/RIU, where $\Delta \lambda$ is the corresponding central wavelength shift of the resonant dips, and $\Delta n$ is the difference of the refractive index. When the fluid (or molecular) system is resonant with the Au thin film with the air-holes arrays, the transmittance spectrum is strongly modified, showing characteristics of strong exciton-plasmon coupling and leading to a bonding resonant mode [12]. This observation can be understood based on the analysis of the planar waveguide propagation constant, i.e., a small change in the $\lambda_{res}$ leads to a large change in the propagation constant. The significant shift of the transmission resonance can be used to monitor changes in the surrounding media [13-15]. This feature provides a remarkable scheme of nanoscale sensing for the RI variations of the environmental medium such as applications in liquid and gas sensing.

4. Conclusion
The optical properties of a 2-D periodic array of sub-wavelength air-holes array in an Au thin film are investigated by using 3-D FEM. The analysis shows that there exists a strong resonance peak in the transmission spectrum of the structure ranging from the visible to near-infrared spectral region. The calculations show that the transmission resonance is a geometric effect resulting from the constructive interference of RLW modes propagating within the air-holes array in an Au thin film. Results show that the geometrical parameters of the structure considerably affect the transmission spectrum. By decreasing the thickness of the air-holes array in the Au thin film, the $\lambda_{res}$ can be shifted from 100 nm to 400 nm. Thus the transmission spectrum can be elastically tailored for various applications. We have shown that the position of the transmission resonance depends strongly on the RI of the medium within the circumference of the air-holes in the Au thin film. This effect can be used in applications including sensors, imaging, and the detection of, e.g. biomolecules and nanophotonic devices.

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