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Xiangnan Zhang

Guiqiang Liu

Zhengqi Liu

Zhengjie Cai

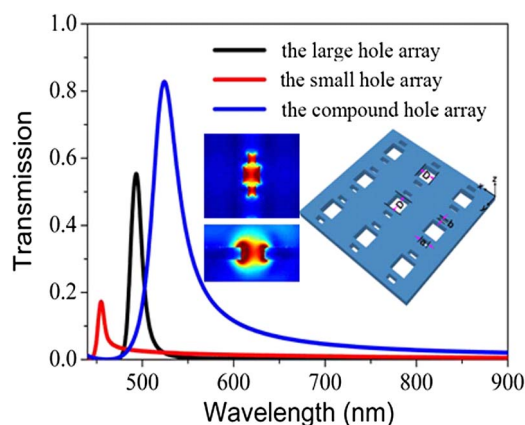
Ying Hu

Xiaoshan Liu

Guolan Fu

Huogui Gao

Shan Huang



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Xiangnan Zhang, Guiqiang Liu, Zhengqi Liu, Zhengjie Cai, Ying Hu, Xiaoshan Liu, Guolan Fu, Huogui Gao, and Shan Huang

Laboratory of Nanomaterials and Sensors, College of Physics and Communication Electronics, Jiangxi Normal University and Key Laboratory of Optoelectronic and Telecommunication of Jiangxi Province, Nanchang 330022, China

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Abstract: The optical transmission properties of the metallic film with an array of compound rectangular nanoholes are numerically investigated by the finite-difference time-domain (FDTD) method. The compound rectangular nanohole (unit cell) in such a structure consists of a large square hole with two small rectangular holes symmetrically distributed at its both sides. Extraordinary optical transmission (EOT) of more than 85% is obtained in this structure, which is larger than that found in the metal film perforated only with the large hole array (55%) or the small hole array (18%). The EOT in the optical regime mainly results from the excitation and coupling of localized surface plasmon resonances and surface plasmon polaritons. The EOT properties can be efficiently tailored in both wavelength and transmission intensity by varying the size and shape of nanoholes. Our structure also shows the sensitivity to environmental dielectric constant. These results indicate that our structure has potential applications in plasmonic filters and sensors.

Index Terms: Enhanced optical transmission, local surface plasmon resonances, sensors, compound rectangular holes.

1. Introduction

In metallic systems, conduction electrons undergo plasmon oscillations and can propagate along the metal surface at optical frequencies due to the excitation of surface plasmon polaritons (SPPs) or localized surface plasmon resonances (LSPRs) [1]–[6]. Enhanced optical transmission (EOT), since firstly being found in the metal film perforated with subwavelength hole arrays, has attracted lots of attention due to its potential applications in optoelectronic field [7], [8]. Originally, the excitation of SPPs has been believed to be one main reason for EOT due to the match between the wavelength of SPPs and the period of aperture arrays [3]. Recently, LSPRs have also been found to play an important role on EOT [9], [10] in metal nanostructures with periodic hole arrays such as circular, rectangular, triangular, and compound holes due to their unique properties such as the capability of overcoming the diffraction limit, miniaturized size, and strong optical field confinement [11]–[13]. So far, many devices based on LSPRs or

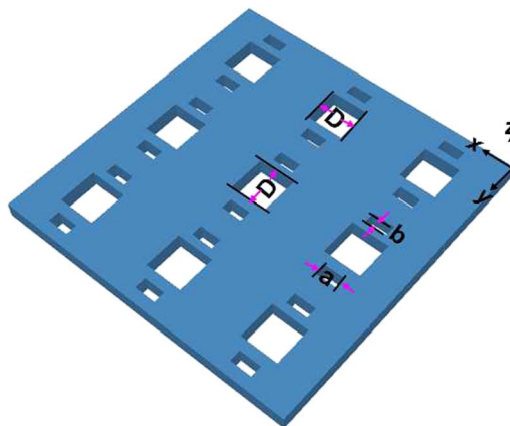


Fig. 1. Schematic diagram of the metal film perforated with a compound nanohole array.

SPPs have been realized both theoretically and experimentally, such as plasmonic filters, sensors, and waveguides [14]–[17]. However, many nanostructures with simple hole arrays can't obtain high transmission or can't realize the consistence between the simulation and experiment in the optical regime. Metallic nanostructures with compound holes generally offer higher coupling efficiency than those with simple circular or rectangular apertures due to the excitation and coupling of LSPRs and SPPs [18]–[23]. For example, Wang *et al.* have obtained perfect transmission in the gigahertz region via a structure of double sets of circular holes arranged into a rectangular array [20]. Liu *et al.* have achieved the tunable high optical transmission in the compound subwavelength hole arrays [18]. However, the fabrication of metallic nanostructures with complicated compound holes is usually difficult, which greatly limits their practical applications. Therefore, metallic nanostructures with simple compound hole arrays, which are easy to realize, are more desired to achieve the tunable and prominent EOT for the applications in integrated nanophotonic circuits and optoelectronic devices.

In this paper, a simple metallic nanostructure consisting of a silver (Ag) perforated with an array of compound rectangular holes is theoretically proposed and investigated by using three-dimensional finite-difference time-domain (FDTD) method. The compound rectangular nanohole in such a structure consists of a large square hole with two smaller rectangular holes symmetrically distributed at its both sides. Due to the employment of symmetrical small rectangular holes at both sides of the large holes with nanometer's separated distance, strong near-field coupling of LSPRs appears. As a result, EOT with more than 90% transmission intensity is obtained in the visible region, larger than those observed in the metallic nanostructures perforated with conventional hole arrays but without considering the near-field coupling effect of LSPRs [7], [8]. The obtained EOT mainly originates from the excitation of LSPRs in the nano-holes and SPPs on metal surface and the strong near-field coupling of LSPRs [9], [10], [18]. In addition, obvious optical responses to the structure parameters and environmental refractive index suggest the tunability and sensitivity of EOT property in our proposed structure. These findings imply that our structure has potential applications such as plasmonic filters and sensors.

2. Structure Model and Simulations

The proposed structure is shown in Fig. 1. The compound nanohole array consists of a large square hole and two small rectangular holes symmetrically distributed at its both sides along the y direction. SiO_2 is selected as the substrate material due to its high transparency. The size of the square holes is D . The length and width of the rectangular apertures are a and b , respectively. The period (p) of the hole array and the thickness of metal film are fixed to 400 nm (except special statement) and 50 nm, respectively. The distance between the center positions

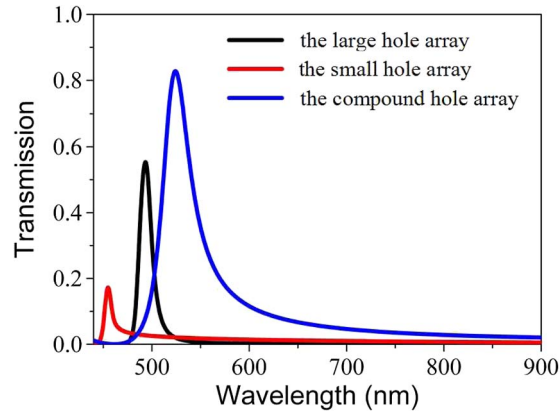


Fig. 2. Transmission spectra of the Ag films perforated with the large hole array, the small hole array, and the compound hole array. Here, $D = 100$ nm, and $a = b = 50$ nm.

of the large hole and the small hole in a unit is 100 nm. Ag with a good conductivity is selected as the metallic material, whose frequency dependent permittivity $\varepsilon(\omega)$ is characterized by the Drude model, which is given as

$$\varepsilon_{\text{Ag}} = 1 - \omega_p^2 / [\omega(\omega + i\gamma)] \quad (1)$$

where the plasma frequency $\omega_p = 2\pi \times 2.175 \times 10^{15} \text{ s}^{-1}$, and the damping constant $\gamma = 2\pi \times 4.36 \times 10^{12} \text{ s}^{-1}$ [24]. The FDTD method is employed to calculate the optical properties. The structure is illuminated by a plane wave with electric field along the x direction at normal incidence. The light resource is placed 250 nm from the structure. The calculation converge satisfies a mesh size of 3 nm. The region is truncated by periodic boundary conditions along the x and y directions and perfect matched layers along the z direction. All transmission spectra were normalized by the incident light intensity.

3. Results and Discussion

Firstly, we investigated the transmission spectra of the metal films respectively perforated with the large hole array (square holes with size of D , black line), the small hole array (square holes with size of a , red line), and the compound hole array proposed in this work (blue line), as shown in Fig. 2. Here, $D = 100$ nm, $a = b = 50$ nm, and $p = 400$ nm. As reported in our previous work [19], the Ag film with 50 nm in thickness is opacity to light. After perforating the Ag film with nanoholes, obvious transmission enhancement in the optical regime is observed in these three structures. When there is a small hole array (or a large hole array) in the Ag film, the maximum transmission intensity is 18% (or 55%). Surprisingly, by integrating the large and small holes together as shown Fig. 1, the transmission intensity is largely enhanced. The maximum transmission (85%) is even larger than the sum of those of the two structures mentioned above, indicating that our proposed structure in Fig. 1 can offer higher coupling efficiency. As reported before, for the metal film perforated with an array of apertures under normal incidence, the excitation of SPPs on metal film surface contributes to the EOT phenomena [1]. The excitation of SPPs can directly couple light into the structures and then further excite the LSPRs at the edges of holes [9]. The excited LSPRs in the nanoholes can transfer the energy from the top surface to the bottom surface of the structure and then re-radiate at the opposite film interface [23]. The nanoholes in such structures can also be regarded as Fabry-Férot (FP) resonant cavities with both ends open [21]. When the spread of surface plasmons satisfies a certain phase condition, the holes achieve maximum transmittance [21]. For the Ag film perforated with the simple rectangular hole array, the interaction between adjacent holes can be ignored due to the large distance between them [3]. Therefore, their low transmission intensities observed in Fig. 2 mainly

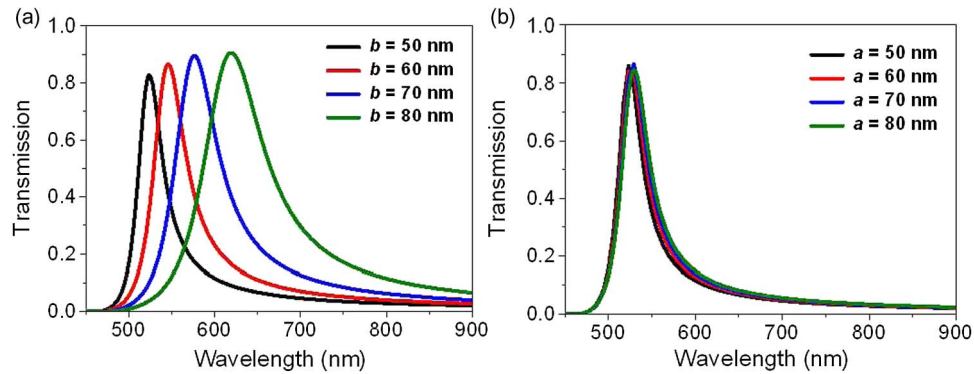


Fig. 3. Transmission spectra of the proposed structure (a) with different b and fixed $a = 50$ nm and (b) with different a and fixed $b = 50$ nm. Here, $D = 100$ nm.

originate from the excitation of SPPs on metal surface and LSPRs in nanoholes and the FP resonant effects of holes. While for the proposed structure, the nanometer's separated distance between the adjacent large and small holes (25 nm) contributes to the near-field coupling of LSPRs between them. Therefore, it can be concluded that the strong near-field coupling of LSPRs between the large and small holes results in the largely enhancement of transmission intensity of the proposed structure, which might provide promising applications in integrated optoelectronic devices.

In order to understand the physical mechanism of the EOT obtained in the proposed structure, we then focused on the effects of nanohole sizes on the transmission spectra. Fig. 3(a) shows the transmission evolution process by varying the width (b) of small rectangles. Here, $D = 100$ nm, $a = 50$ nm. The transmission peak shows a red-shift from 522 nm to 617 nm with b increasing from 50 to 80 nm with a step of 10 nm, accompanied by an increased intensity from 85% to 92%. As b increases from 50 nm to 80 nm, the Ag spacer thickness between the adjacent large and small holes decreases from 25 nm to 10 nm in intervals of 5 nm, which leads to the strengthened near-field coupling of LSPRs. The strengthened near-field coupling of LSPRs contributes to the enhancement of transmission and the red-shift of transmission peak [23], [25]. This again demonstrates the important role of near-field of LSPRs between adjacent holes on the enhanced transmission.

Fig. 3(b) shows the transmission evolution process by varying the length (a) of small rectangles from 50 nm to 80 nm. Here, $D = 100$ nm, $b = 50$ nm. However, no obvious change is observed here. The intensity and position of the transmission peak are nearly invariable as a increases. It is worth noting that the thickness of the Ag spacer between the neighboring large and small holes is invariable whatever the length a changes. The unchanged Ag spacer thickness indicates the near-field coupling of LSPRs between the neighboring large and small holes in the y direction almost remains the same. Since SPP and LSPR modes mainly propagate along the x direction when illuminated by the plane wave with electric field along the x direction, their resonant conditions would not be affected by the change of a [18]. As a result, the spectral properties of the proposed structure do not change under this condition.

Fig. 4(a) and (b) show the normalized electric field intensity $|E|^2$ distribution patterns for the peak at $\lambda = 545$ nm in the xoy and xoz planes ($z = 25$ nm), respectively. Here, $|E|^2 = E_x^2 + E_y^2 + E_z^2$, $D = 100$ nm, and $a = b = 60$ nm. Weak electric field intensity is found on the surface of the metal film, which confirms the excitation of SPPs. The excitation of SPPs contributes to the coupling of light into the structure and the further excitation of LSPRs in the holes. Extremely strong electric field energy confined at both sides of all holes along the x direction confirms the excitation of two kinds of LSPRs (large and small holes' plasmon modes). When surface plasmons in the hole satisfies a certain phase condition, LSPRs excited at the ridges of nanoholes would act as efficient dipole scatterers re-emitting the incident light along the z direction [9]. The

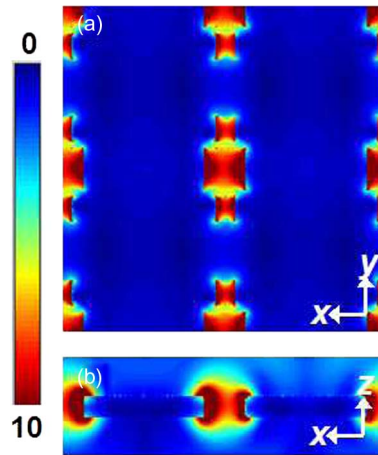


Fig. 4. Normalized electric field intensity $|E|^2$ distributions of the structure in the xoy (a) and xoz (b) planes ($z = 25$ nm) at $\lambda = 545$ nm. Here, $D = 100$ nm, and $a = b = 60$ nm.

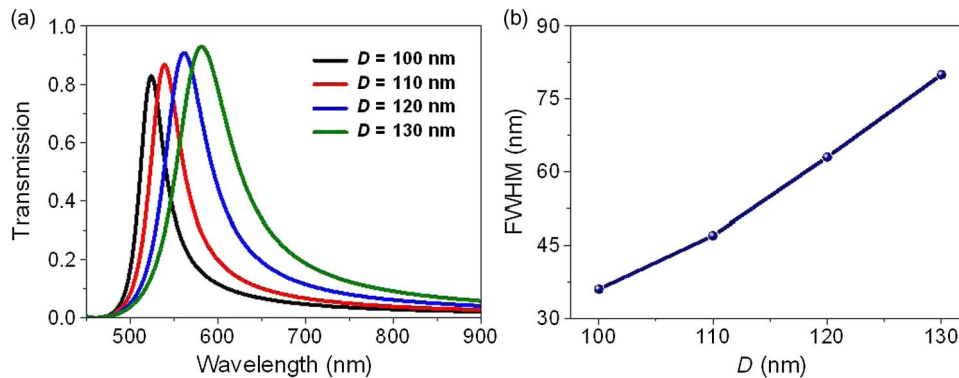


Fig. 5. (a) Transmission spectra of the structure with different D . (b) FWHM of the structure as a function of D . Here, $a = b = 50$ nm.

efficient light coupling input and output effects at the two entrances of nanoholes are clearly observed in Fig. 4(b). Similar to the plasmon hybridization model, the resonant plasmon mode in the compound hole arrays would be generated by the coupling and interaction of the large and small holes' plasmon modes [22]. Strong electric field energy confined between the adjacent large and small holes in Fig. 4(a) demonstrates the appearance of strong near-field coupling of LSPRs between them. The strengthened coupling and hybridization of LSPRs are closely related to the red-shift of transmission spectra shown in Fig. 3(a) [23]. Therefore, the excitations of SPPs and LSPRs together with the near-field coupling effects of LSPRs are the main reason for the EOT phenomenon observed in our proposed structure.

Inspired by the optical properties obtained above, we further studied the role of the size (D) of square holes on transmission spectra, as shown in Fig. 5(a). Here, $a = b = 50$ nm. Similar to those observed in Fig. 3(a), the transmission peak shows an obvious red-shift and an approximately linear increase in intensity. The maximum transmission value even reaches up to 94% at $\lambda = 590$ nm with the semi-transparent (transmission $> 50\%$) bandwidth over 80 nm, which is higher than that of the structure with a compound symmetric arrangement of hole array reported in [18]. It is because that when the size of the large holes increases from 100 nm to 130 nm, the thickness of the Ag spacer between the adjacent large and small holes decreases from 25 nm to 10 nm. The decreased distance could lead to the strengthened near-field coupling of LSPRs and thus results in the enhanced intensity and red-shift of transmission peak [23]. The full width

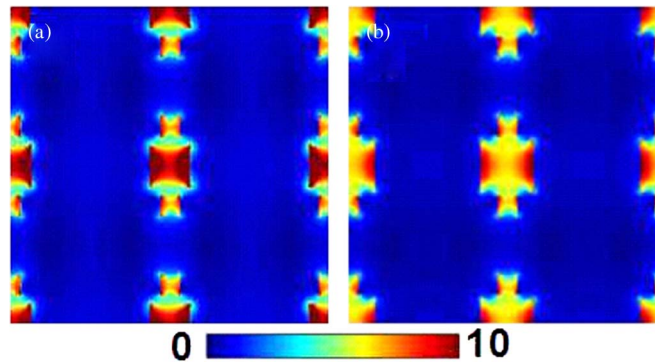


Fig. 6. Normalized electric field intensity $|E|^2$ distributions of the structure with $D = 100$ nm at $\lambda = 522$ nm (a) and $D = 130$ nm at $\lambda = 581$ nm (b) in the xoy plane ($z = 25$ nm). Here, $a = b = 50$ nm.

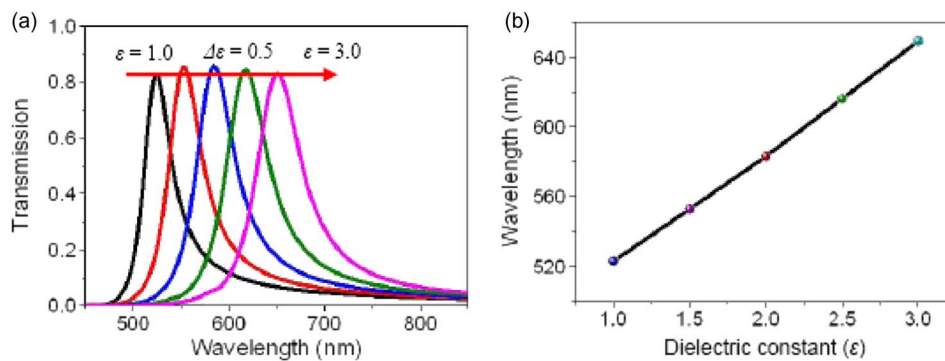


Fig. 7. (a) Transmission spectra as a function of environmental dielectric constant (ϵ). (b) Peak positions as a function of dielectric constant ϵ . Here, $a = b = 50$ nm, and $D = 100$ nm.

at half maximum (FWHM) of the proposed structure with different D is depicted in Fig. 5(b). An approximately linear increase from 36 nm to 80 nm is observed as D changes, originating from that the increased size of large holes contributes to larger oscillations for LSPRs.

Fig. 6 presents the normalized electric field intensity $|E|^2$ distributions of the structure with $D = 100$ nm at $\lambda = 522$ nm (a) and $D = 130$ nm at $\lambda = 581$ nm (b) in the xoy plane. Here, $a = b = 50$ nm. Obviously, stronger field energy occurs between the adjacent large and small holes when D increases, which implies the enhanced near-field coupling of LSPRs between them. The strengthened near-field coupling of LSPRs results in the enhanced intensity and the red-shift of transmission peak as Fig. 5(a) shown. Compared with Figs. 4 and 6(a), the electric field energy in Fig. 6(b) shows more uniform distribution, indicating larger oscillations for LSPRs as D increases which contribute to a larger FWHM, as shown in Fig. 5(b).

We also investigated the optical properties of the proposed structure by changing its environmental dielectric constant (ϵ) with fixed parameters ($a = b = 50$ nm, $D = 100$ nm). The uniform red-shift of the resonant peak from 522 nm to 650 nm with almost unchanged bandwidth and intensity is observed as ϵ increases from 1.0 to 3.0 in intervals of 0.5 (see Fig. 7(a)), suggesting the optical sensitivity of the proposed scheme to different dielectric surroundings. A linear enhancement of resonant wavelength is found (Fig. 7(b)). The calculated sensitivity of the proposed structure to refractive index variation ($n = \epsilon^{1/2}$) is 178 nm/RIU (refractive index unit). This result indicates that our structure can also be used for deep sub-wavelength plasmonic sensors.

Finally, we also investigated the effect of the period (p) on the optical transmission behaviors, as shown in Fig. 8. For the Ag film perforated with the hole array, the peak positions λ_{\max} ,

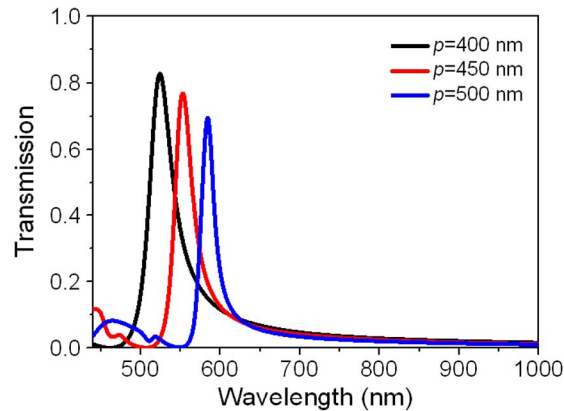


Fig. 8. Transmission spectra as a function of period p .

originating from the activation of SPP modes, are given in a first approximation by the following equation [9]:

$$\lambda_{\max} = \frac{p}{\sqrt{i^2 + j^2}} \sqrt{\frac{\varepsilon_d \varepsilon_m}{\varepsilon_d + \varepsilon_m}} \quad (2)$$

where p is the period, i, j are integers defining the different diffraction orders, and ε_d and ε_m are the dielectric constants of the interface medium and metal, respectively. Equation (2) clearly shows that the period and dielectric constants have direct influences on the wavelength peak position. With the environment dielectric constant increasing, the red-shift of wavelength peak appears in our proposed structure as shown in Fig. 7, well agreement with this equation. According to (2), the resonant wavelength peak would show an identical trend as p changes. In Fig. 8, it is clearly observed that when p increases from 400 nm to 500 nm, the transmission peak shows an obvious red-shift from 522 nm to 600 nm, accompanied by a slight decrease in transmission intensity. Therefore, the EOT phenomenon found in our proposed structure can be attributed to the excitations of SPPs on metal film surface and the LSPRs relying on nanoholes and the strong near-field coupling of LSPRs.

4. Conclusion

In summary, we have theoretically studied the optical transmission properties of a metal film perforated with a periodic compound rectangular nanohole array. An enhanced transmission peak with high transmission and narrow bandwidth is obtained due to the excitation of LSPRs in the nanoholes and SPPs on the metal surface and the strong near-field coupling of LSPRs between the adjacent large and small holes. The EOT properties can be efficiently tailored by varying the parameters including the size and shape of holes. In addition, the resonant frequency of our proposed structure is sensitive to the dielectric constants of surrounding environment. These results suggest that our proposed structure has potential applications in optoelectronic devices.

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