The effect of array periodicity on the filtering characteristics of metal/dielectric photonic crystals

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Abstract: We present a both theoretical and experimental investigation into the effect of array periodicity on the filtering characteristics of metal/dielectric photonic crystals (MDPhCs) with hexagonal arrays of subwavelength holes in gold/silicon dioxide films, varying the array periodicity from 6 to 8 μ m every 1 μ m while the ratio of hole radius to array periodicity is kept constant (1/4). The results indicate that the reflectance spectrum is highly dependent on the array periodicity. When the array periodicity increases, the reflectance spectrum exhibits a large redshift regularly. The finite difference time domain (FDTD) simulations agree well with the experimental results. By analyzing the relationship between the position of the reflectance minimum and the array periodicity under the conditions of keeping the same ratio of hole radius to array periodicity (1/4). This finding provides an effective way to control the filtering characteristics of MDPhCs, which have potential applications in optical filters, plasmonic thermal emitters and so on.

Key words: optics at surfaces; surface plasmon polaritons; array periodicity; FDTD method; metal/dielectric photonic crystal; filtering characteristic

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1. Introduction

Since the discovery of extraordinary optical transmission (EOT) through subwavelength hole arrays in metal films was reported by Ebbesen and coworkers in $1998^{[1]}$, there has been abundant research activity aimed at understanding the physics and at the many promising applications associated with this phenomenon. The mechanism of EOT is nowadays widely understood in terms of the excitation and coupling of surface plasmon polaritons (SPP) on the metal/dielectric interface^[1-3]. Now, properly controlling the EOT phenomenon is becoming ever more important as applications are developed, such as surface plasmon resonance sensing, tunable filter and plasmonic thermal emitters^[4-6].

The EOT is a complex phenomenon that depends on many parameters, such as the real metal properties^[7], the metal thick-ness^[8], the hole shape and size^[9], and the array periodic $itv^{[10-12]}$. Ebbesen^[1] first illustrated that the positions of transmission peaks scale exactly with the array periodicity, independent of metal (Ag, Cr, Au), hole diameter and film thickness. Recently, the influence of array periodicity on the EOT has generated considerable interest. This is because the metallic hole array acts like a tunable filter by changing the array periodicity simply. For example, Thio^[10] reported a systematic study of the effects of parameters on zero-order transmission spectra with the same array periodicity but different hole diameters and with the same hole diameter but different array periodicities. The position of the transmission peak depends partly on the hole size but mainly on the array periodicity. Those works focused on the situation in which either the array periodicity or the hole diameter was changed respectively. As a result, they did not separate the contributions of the array periodicity and hole diameter.

The filtering effect of hole arrays in a metal film has been considered for thermal emitters recently. Puscasu *et al.*^[13] and Pralle *et al.*^[14] discovered that the MDPhC has extraordinarily sharp thermal emission that substantially modifies the blackbody spectrum. It was demonstrated that the array periodicity mainly determines the position of the narrow band thermal emission wavelength. Xiao *et al.*^[15] discovered that the effect of the ratio of hole radius to array periodicity on EOT characteristics for MDPhCs with hexagonal round hole arrays, it was demonstrated that with the ratio being 1/4, a narrow bandwidth and high efficiency transmission is achieved.

In this work, we will present our experimental and theoretical investigations on filtering characteristics for MDPhC with hexagonal round hole arrays in optically thin gold/silicon dioxide films by changing the array periodicity yet the ratio of hole radius to array periodicity being 1/4. These experimental results are in good agreement with the theoretical simulations based on FDTD calculations.

2. Experimental section

Figure 1 is a schematic diagram of a Au/SiO₂ photonic crystal with a hexagonal array of round holes residing on the Si substrate in side view. In this experiment, three different samples were fabricated, and the array periodicity and the round hole diameter of the hexagonal arrays were 6, 7, 8 μ m and 3, 3.5, 4 μ m, respectively. The sample fabrication processes of the Au@SiO₂@Si MDPhC are described as follows. (1) A layer of silicon dioxide ($d_2 = 0.5 \mu$ m) was deposited by ther-

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Fig. 1. Schematic diagram of the Au@SiO₂@Si MDPhC structure with hexagonal round hole arrays in side view. The top view of the experimental structure is shown at top right.

mal oxidation on the front side of the p-doped single-polished silicon wafers. (2) Another thin Au film ($d_1 = 0.1 \ \mu m$) was deposited by sputtering on the front side of the SiO₂ @ Si substrate. (3) The three samples were followed by three different array periodicities ($a = 6, 7, 8 \mu m$) and three different round hole diameters ($2r = 3, 3.5, 4 \mu m$). Finally, the air round hole hexagonal arrays were etched through a Au/SiO2 structure into the silicon substrate to a total depth of 7 μ m ($d_1 + d_2 + d_3$) by using a lithography process with reactive ion etching (RIE). Each set of samples keeps the same structural parameters consisting of d_1, d_2 and d_3 , and the total array area is approximately $2 \times 2 \text{ mm}^2$. The three experimental samples were characterized by an electron microscope. The electron micrograph of the top view of the experimental structure is shown in the top right of Fig. 1. The round hole hexagonal arrays were well defined, and the surfaces of the samples were smooth, which indicated that the obtained samples were of high quality. A Fourier transform infrared spectrometer was employed to characterize the reflectance spectra of the samples (as shown in Fig. 2).

3. Results and discussion

Figure 2 shows the reflectance spectra at normal incidence for Au@SiO₂@Si MDPhC with hexagonal round hole arrays as a function of array periodicity ($a = 6, 7, 8 \mu m$) with the ratio (r/a) being 1/4. We find that both the position (λ_{\min}) of the reflection minimum (dip) and the bandwidth ($\Delta\lambda$) appear to be strongly dependent on the array periodicity (a). As we know, the expression of absorptivity is A = 1 - R - T. Yet, the measured transmission (T) is close to 0. Hence, $A \cong 1 - R$. An absorption peak is then equivalent to a reflectance dip. If the Si substrate was very thin, the reflection minimum would correspond to a transmission peak. So, we can estimate the filtering characteristics for the MDPhC structure by three key parameters (λ_{\min} , $\Delta\lambda$ and $\Delta\lambda/\lambda_{\min}$). When the array periodicity increases from 6 to 7 to 8 μ m with the ratio (r/a) being 1/4, the position of the reflectance dip regularly redshifts from 5.85 to 6.76 to 7.73 μ m. The redshift of λ_{min} with the increase in



Fig. 2. Measured reflectance spectra of Au@SiO₂@Si MDPhC as a function of array periodicity ($a = 6, 7, 8 \mu m$) with the ratio (r/a) being 1/4.

the array periodicity results from the coupling of SPP at the air/gold interface^[2]. Simultaneously, the bandwidth of the reflectance dip regularly increases from 0.38 to 0.53 to 0.57 μ m. The augment of $\Delta\lambda$ with the increase in the array periodicity results from the different ratio ($-\varepsilon_{\rm rm}/\varepsilon_{\rm im}$) of the negative real to the imaginary of gold film permittivity under three different resonant wavelengths (5.85, 6.76 and 7.73 μ m), which largely determine the bandwidth^[7, 10]. In addition, the ratio ($\Delta\lambda/\lambda_{\rm min}$) of bandwidth to the position of the reflection dip is 0.06, 0.07 and 0.07, respectively. All of these values are very small as well as almost being the same. That is to say, the MDPhC structure with hexagonal round hole arrays by changing the array periodicity yet the ratio (r/a) being 1/4 exhibits a good filtering characteristic.

To elucidate the dependence of λ_{min} on the array periodicity, we can introduce a method to predict the positions of transmission peaks in the EOT phenomenon. This can be understood by considering the SPP coupling with the incident light. In the case of hexagonal round hole arrays, at normal incidence, the position of the reflectance minimum is given by^[10]

$$\lambda_{\min} = a \left[\frac{4}{3} \left(i^2 + ij + j^2 \right) \right]^{-1/2} \left(\frac{\varepsilon_{\rm d} \varepsilon_{\rm m}}{\varepsilon_{\rm d} + \varepsilon_{\rm m}} \right)^{1/2}, \quad (1)$$

where $\varepsilon_{\rm m}$ and $\varepsilon_{\rm d}$ are the dielectric constants of the metal and the adjacent medium, and *i* and *j* are integers. In the wavelength range of our experiments, the dielectric constants of gold and air are $\varepsilon_{\rm Au} \approx -3.3 \times 10^3 + 5.9 \times 10^2 i^{[16]}$ and $\varepsilon_{\rm air} = 1$, respectively. With the array periodicity being 6, 7, 8 μ m, $\lambda_{\rm min}$ corresponds to the SPP modes $(i, j) = (\pm 1, 0)$ and $(0, \pm 1)$ at the air/gold interface are calculated as 5.2, 6.06, 6.93 μ m, respectively. The calculated positions have some slight difference is because the calculated values are obtained by assuming that the structured metal films are continuous^[2].

To achieve an in-depth understanding of the effect of array periodicity on the filtering characteristics of MDPhC, we used a 3D finite difference time domain (FDTD)^[17] numerical simulation to model the reflectance spectra of Au@SiO₂@Si MD-PhC with hexagonal round hole arrays as a function of array periodicity ($a = 6, 7, 8 \mu m$) with the ratio (r/a) being 1/4. We



Fig. 3. FDTD calculated reflectance spectra of Au@SiO₂@Si MD-PhC as a function of array periodicity ($a = 6, 7, 8 \mu m$) with the ratio (r/a) being 1/4.

used periodic boundary conditions associated with the hexagonal round hole structure and absorption conditions to truncate the directions parallel to the Au film surface. Yet, the incident light is vertical to the Au film surface. All of the structure parameters are the same as in the experiment. The response of the Au film layer was captured using the standard Drude model, and the wavelength dependent permittivity of Au was taken from Ref. [16]. Using a uniform 4 nm grid size, we integrated with 6.5 attosecond time-steps for a duration of 106 fs and calculated the resulting reflectance (as shown in Fig. 3).

Figure 3 shows the FDTD calculated reflectance spectra at normal incidence for Au@SiO2@Si MDPhC with hexagonal round hole arrays as a function of array periodicity (a = 6, 7,8 μ m) with the ratio (r/a) being 1/4. We also find that both λ_{min} and $\Delta\lambda$ appear to be strongly dependent on the array periodicity. The FDTD simulation results show good agreement with the experimental results presented in Fig. 2 for the same conditions. When the array periodicity increases from 6 to 7 to 8 μ m with the ratio (r/a) being 1/4, the λ_{\min} redshifts from 5.96 to 6.68 to 7.6 μ m. The redshift of λ_{min} with the increase in the array periodicity results from the coupling of SPP on the air/gold interface. Simultaneously, $\Delta\lambda$ regularly increases from 0.78 to 0.96 to 1.09 μ m. The augment of $\Delta\lambda$ with the increase in the array periodicity can be illuminated according to the different ratio $(-\varepsilon_{\rm rm}/\varepsilon_{\rm im})$ of the negative real to the imaginary of gold film permittivity with three different resonant wavelengths (5.96, 6.68 and 7.6 μ m). In addition, $\Delta\lambda/\lambda_{min}$ is also so small as 0.13, 0.14 and 0.14, respectively. It is demonstrated that the MDPhC structure with hexagonal round hole arrays by changing the array periodicity yet the ratio (r/a) being 1/4 also exhibits a good filtering characteristic according to the FDTD calculation. Theoretical analysis of the results would also be useful to gain a better insight into these filtering characteristics. Perhaps only then can we expect to grasp the full implications of these findings.

For a better comparison, we have plotted three curves based on the experimentally measured FDTD calculated and SPP coupling theory calculated data. The relation between the position (λ_{min}) of the reflection dip and the array periodicity (*a*) is shown in Figure 4. We clearly saw SPP coupling assisted filtering characteristics for the Au@SiO₂@Si MDPhC



Fig. 4. Experimentally measured and FDTD calculated position λ_{\min} of the reflection dip as a function of array periodicity *a*. The inset shows the SPP coupling theory calculated position λ_{\min} of the reflection dip corresponds to the SPP modes $(i, j) = (\pm 1, 0)$ and $(0, \pm 1)$ at the air/gold interface as a function of array periodicity *a*.

with hexagonal round hole arrays by changing the array periodicity yet the ratio (r/a) being 1/4, which is in excellent agreement with our experimental results and the FDTD simulation results. The linear relationship between the array periodicity (a) and the position (λ_{\min}) of the reflection dip becomes obvious. λ_{\min} can be fitted using a linear function to determine the filtering characteristics for MDPhC with hexagonal round hole arrays. The fitting curve of the FDTD simulation results is $\lambda_{\min} = 1 + 0.82a$. The fitting curve of the experimental results is $\lambda_{\min} = 0.2 + 0.94a$. Both the relationship by fitting the FDTD simulation results and the relationship by fitting the experimental results are the same linear relationship basically. The inset (as shown in Fig. 4) shows that the SPP coupling theory calculated position (λ_{\min}) of the reflection dip corresponds to the SPP modes $(i, j) = (\pm 1, 0)$ and $(0, \pm 1)$ at the air/gold interface as a function of array periodicity (a). Using Eq. (1), we can easily deduce a theoretical equation, $\lambda_{\min} \approx \sqrt{3}a/2 = 0.87a$. By comparing the slope (0.82, 0.94 and 0.87) of three different relationships, we find that the change trend of the position (λ_{\min}) of the reflection dip along with varying the array periodicity (a) yet the ratio (r/a) being 1/4 almost is the same. The equation by the introduction of the SPP coupling mechanism is coincident with the former two linear equations, namely it is demonstrated that the SPP coupling mechanism can be used to explain the filtering characteristics of MDPhC.

Both the experimental results and the FDTD simulation results indicate that the SPP coupling assisted filtering characteristics for MDPhC operate, which presents a further development of the EOT studies. In this case, such a system (MDPhC with hexagonal round hole arrays by changing the array periodicity yet the ratio (r/a) being 1/4) has brought new methods for the filtering control of MDPhC. It is proposed that the coupling of the SPP at the air/gold interface is involved in the process. This is because the array periodicity is critical to control the SPP coupling direction of the air/gold interface. When the array periodicity is adjusted, the λ_{min} and $\Delta\lambda$ must be changed regularly. This is a new and fascinating phenomenon to emerge in this work, yet the other research works have no similar report^[1, 10–12]. The physical origin of the observed behavior arises from the separate contributions of the coupling between the normal incident light and the SPP modes at the air/gold interface and the effect of the ratio (r/a) being 1/4 to the enhanced transmission through the SPP evanescent mode of the Au film layer. The evanescent mode is responsible for Bragg resonances in the SPP that allow for enhanced transmission.

4. Conclusion

In conclusion, by varying the array periodicity from 6 to 8 μ m every 1 μ m yet the ratio (r/a) being 1/4 in a MDPhC with hexagonal round hole arrays, we have shown that the array periodicity plays an important role in the filtering control of MDPhC. These experimental results are in good agreement with theoretical simulations based on FDTD calculations. The main findings of our work are summarized as follows. First, the MDPhC with a hexagonal round hole array structure exhibits good filtering characteristics, which can be tuned and scaled by merely adjusting the array periodicity. Second, both the relationship ($\lambda_{\min} = 1 + 0.82a$) by fitting the FDTD simulation results and the relationship ($\lambda_{\min} = 0.2 + 0.94a$) by fitting the experimental results are the same linear relationship basically. Third, at the same time, it is observed that the theoretical equation ($\lambda_{\min} \approx \sqrt{3a/2} = 0.87a$) being calculated by the SPP coupling theory can validate our experimental and simulation results. These findings will be important for designing a MDPhC device for a plasmonic thermal emitter with selective work wavelength that is critical for gas and chemical sensing applications. The work wavelengths are selective, which should be very useful for the creation of a tunable plasmonic thermal emitter with a desirable wavelength by merely adjusting the array periodicity.

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