Enhanced Transmission through Periodic Arrays of Subwavelength Holes: The Role of Localized Waveguide Resonances

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By using the rigid full-vectorial three-dimensional finite-difference time-domain method, we show that the enhanced transmission through a metallic film with a periodic array of subwavelength holes results from two different resonances: (i) localized waveguide resonances where each air hole can be considered as a section of metallic waveguide with both ends open to free space, forming a low-quality-factor resonator, and (ii) well-recognized surface plasmon resonances due to the periodicity. These two different resonances can be characterized from electromagnetic band structures in the structured metal film. In addition, we show that the shape effect in the enhanced transmission through the Au film with subwavelength holes is attributed to the localized waveguide resonance.

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For an idealized aperture in an infinitely thin film with perfect electronic conductivity (PEC), Bethe and Bouwkamp showed the transmission of the normal incidence is proportional to $(r/\lambda)^4$ and higher order terms of (r/λ), where r is the hole radius and λ is the wavelength [1–3]. Therefore, the transmission is very weak through a subwavelength hole. In the case of an aperture in a thick PEC film, the transmission decreases further with exponential dependence on the hole depth when the wavelength of the light is larger than the cutoff wavelength of the hole waveguide by Rayleigh's criterion [4]. Since Ebbesen and co-workers discovered the phenomenon of enhanced transmission through the metallic film with periodic arrays of subwavelength holes in 1998 [5], tremendous attention has been focused to investigate the physical mechanism behind this effect. Many researchers show that the enhanced transmission is attributed to the surface plasmon resonance arising from the surface periodicity [6,7], and should be independent of hole shapes. However, recently Klein *et al.* [8] demonstrated experimentally that there is strong influence of hole shape on the enhanced transmission. It was postulated that this shape effect was the result of localized surface plasmon (LSP) resonances [9,10]. Even so, the role of the shape resonances is not clearly understood. In particular, Degiron *et al.* [10] showed that surface plasmon polaritons due to the periodicity might dominate the transmission spectra. Nevertheless, these results were mainly based on transmission spectra, while the dispersion relations, i.e., the band structures, of the surface states might give better insights into this phenomenon. On the other hand, the enhanced transmission due to the periodicity has been demonstrated in the PEC film with the subwavelength hole array [11]. However, the answer to whether there is the shape effect to the enhanced transmission in the structured PEC film is not clear.

In this Letter, we start with investigating the property of the resonance states by analyzing band structures of the Bloch waves in a PEC film with hole arrays, and also their influence on the enhanced transmission through the holes. Even though a PEC-air interface usually does not support surface plasmon waves, it has been shown that surface confined waves can exist at a PEC surface with an array of the drilled holes. These so-called designed-surface plasmons (DSPs) have many important properties in common with ordinary surface plasmons [12–16]. In fact, for a real metal in the optical regime with a hole array, surface plasmon resonances due to the hole structure and those due to the negative permittivity of the metal cannot be separated [12]. Therefore, the conclusion for the enhanced transmission through the structured PEC film can be naturally extended to the case of a real metal in the optical regime. In addition, the case of hole arrays in an Au film for the optical regime is also investigated.

The phenomena of enhanced transmission through subwavelength apertures in a metallic film are usually characterized by the normalized transmission [5,8–10], defined as,

$$T_{\mathrm{norm}} = \frac{T}{S_{\mathrm{hole}}/S_{\mathrm{cell}}} = \frac{P_{\mathrm{out}}}{P_{\mathrm{in}}} \frac{S_{\mathrm{cell}}}{S_{\mathrm{hole}}}, \quad (1)$$

where $P_{\mathrm{in(out)}}$ is the power flux through in (out) the metal film, S_{hole} is the sum area of the hole(s) in a unit cell, and S_{cell} is the area of a unit cell. T_{norm} should be larger than unity for enhanced transmission.

Consider a free standing PEC film with a thickness of $h = 0.2a$ and a square lattice of rectangular $0.9a \times 0.2a$ air holes as shown schematically in Fig. 1, where a is an arbitrary length unit for normalization and d is the lattice constant. Even though only such a specific example is considered in the present Letter, we have studied many

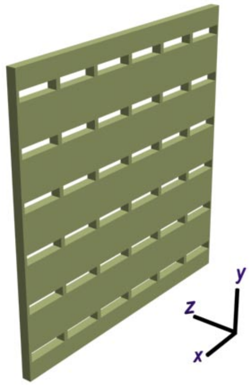
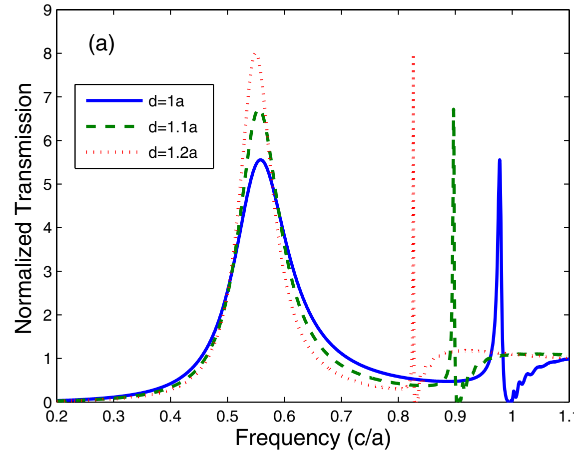


FIG. 1 (color online). The schematic of a perfect conductor film with a square array of rectangular air holes.

different hole shapes and parameters and we find that the results obtained below are general.

The normalized transmission through the film was calculated by the full-vectorial three-dimensional (3D) finite-difference time-domain (FDTD) method [17]. In the present Letter, we only consider the case of normal incidence, and the electric field of the incident wave is polarized along the short edge of the rectangular holes (the y direction). The cases of three different lattice constants: $d = 1.0a$, $1.1a$, and $1.2a$, are investigated here, and the calculation results are shown in Fig. 2(a). In the frequency range shown in the figure, there are two peaks of enhanced transmission at the frequency $0.56(c/a)$ and $0.98(c/a)$ for $d = 1.0a$, where the normalized transmissions are larger than 5.5. When the lattice constant increases while the hole size is fixed, the lower frequency peak does not move significantly while the high-frequency peak is "redshifted" dramatically. The normalized transmissions are still very high and increasing as the lattice constant increases.

To understand this phenomenon clearly, we calculate the dispersion relation (the band structure) of the electromagnetic state for the case of $d = 1.0a$ shown in Fig. 2(b). Since the structure is symmetric about the plane $z = 0$ crossing the center of the film, the resonant modes can be classified as either the odd or even modes where E_z field is antisymmetric or symmetric about $z = 0$. The resonant frequencies corresponding to the Bloch wave vector $\mathbf{k} = \mathbf{0}$ [Γ point in Fig. 2(b)] coincide with the peaks of the normalized transmission [cf. Fig. 2(a)]. Here we consider the bands in the light cone [the white region in Fig. 2(b)], which are the electromagnetic states radiating into free space. Note that if each air hole is considered as a truncated rectangular waveguide with four PEC walls and two sides opened to free space, the truncated waveguide forms a low-Q (quality factor) cavity resonator. The resonant frequency of the lowest-order cavity mode is the same as the cutoff frequency of the basic mode (TE_{10}) in the rectangular waveguide, $0.556(c/a)$. This resonant frequency is almost independent of the periodicity, and gives a flat band in



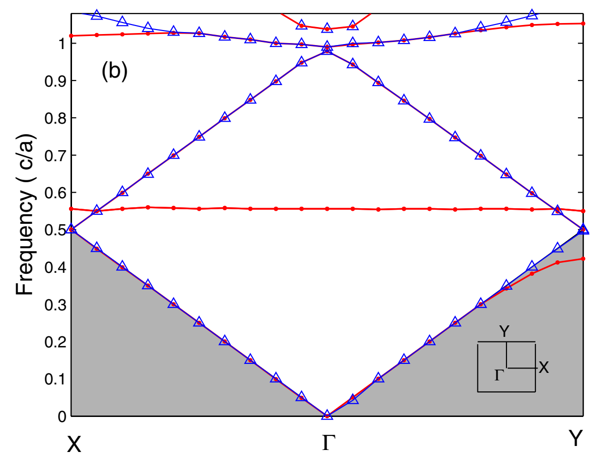


FIG. 2 (color online). (a) The normalized transmission through a PEC film with a square array of rectangular holes of size $0.9a \times 0.2a$ (a is an arbitrary length unit) for different lattice constants: $d = 1.0a$ (solid line), $1.1a$ (dashed line), and $1.2a$ (dotted line). The thickness of the film is $0.2a$. (b) The band structure for the case of the lattice constant $d = 1.0a$. The odd (even) mode is denoted by the line marked with points (triangles). The white area is the region in the light cone.

the electromagnetic band structures, as shown in Fig. 2(b). We refer to this kind of resonance as *the localized waveguide resonance*, and the flat band is a signature of these resonances associated with each air hole. Additionally, it is observed that for the above two-dimensional periodic structure, the localized waveguide resonances always exist even if the metal film is very thin (considering that the thickness of the metallic films is less than the long axis of air holes). This differs from the case of one-dimensional periodic structures, e.g., a metallic grating with slits [7]. To understand this property, a typical Fabry-Perot expression can be used to model the zero-order transmission coefficient (t_{00}):

$$t_{00} = \frac{t_{ah} \exp(-i\beta h) t_{ha}}{1 - r_{ha}^2 \exp(-i2\beta h)}, \tag{2}$$

where t_{ah} is the transmission of the incident wave impinging from free space onto the semi-infinite rectangular waveguide, t_{ha} (r_{ha}) is the transmission (reflection) of the waveguide mode from the semi-infinite rectangular waveguide into free space, and β is the propagation constant of waveguide mode. Since the resonance frequency is very close to the cutoff frequency, β is approximately equal to 0, meaning that both $\exp(-i\beta h) \approx 1$ and $\exp(-i2\beta h) \approx 1$. Therefore, t_{00} is almost independent of h, and the transmission peaks do not change with h, even if the PEC film is very thin.

Now let us consider the second band in the light cone. In the optical regime, the mechanism for enhanced transmission through real metal films patterned with arrays of holes has been well recognized as arising from the surface plasmons [6,7,10]. The periodicity in the array allows the light impinging on the metal to excite the Bloch state with the main component of surface wave on both surfaces of the metallic film. This Bloch state can be reemitted freely into propagating light on the exit side. Meanwhile, the photonic band of the Bloch surface states is folded by the boundary of the first Brillouin zone. The resonant frequencies at the Γ point are thus a function of the lattice constant. In particular, the first resonant frequency is always around the frequency c/d. Therefore, the transmission peak position corresponding to this resonant frequency shall change with the lattice constant, which coincides with our transmission calculation results [cf. Fig. 2(a)]. It is worth noting that the zero transmission at the wavelength corresponding to the lattice constant (i.e., at the frequency $c/d = 1$) is due to the Wood's anomaly [11].

To verify that the frequency of the localized waveguide resonance is mainly determined by the holes size and almost independent of the periodicity, we calculate the transmission through PEC films where the same size holes ($0.9a \times 0.2a$) are randomly distributed with the long axis of the holes always along x direction. Figure 3 shows the normalized transmission for four different calculation square cell sizes: $(5a)^2$, $(7a)^2$, $(9a)^2$, and $(11a)^2$. The spectrums are obtained by the mean value of five different samples for each cell size (a further increase of the number of samples almost has no influence on the mean value). To maintain consistency in the comparison with the film with a periodic array (the solid line in Fig. 3), the ratio of the total holes area to the total cell area is equal to that in the case of the periodic array, i.e., there are N^2 holes in the $(Na)^2$ metallic film (e.g., the inset plots the positions of 25 holes in a $5a \times 5a$ example). It is clear from Fig. 3 that the random distribution of holes maintains a peak position of the transmission near the frequency $0.56(c/a)$, but removes the higher frequency peak at the frequency $0.98(c/a)$ in the case of the periodic array of holes. This confirms that the localized waveguide resonance results from the electromagnetic field localized in the each hole and the surface plasmon resonance is due to the periodicity.

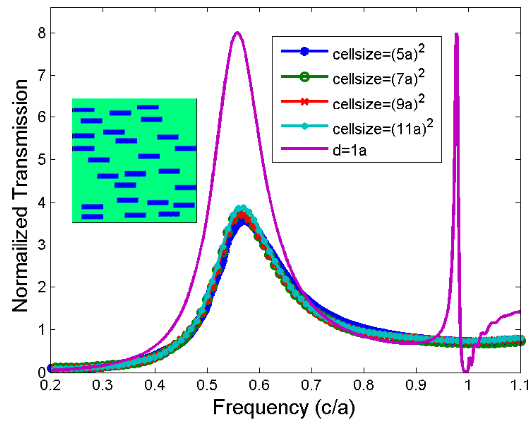


FIG. 3 (color online). The mean value of the normalized transmission for the sample with different square cell size: $(5a)^2$, $(7a)^2$, $(9a)^2$, and $(11a)^2$. For the comparison, the normalized transmission for the case of the periodic array of holes (the lattice constant $d = 1.0a$) is denoted by the solid line. The ratio of the hole area to the cell area in the case of random distributed holes is equal to that in the case of the periodic array. The inset shows an example of 25 randomly distributed holes in a $5a \times 5a$ cell.

The mean value of the normalized transmissions in the case of randomly distributed holes is also larger than 3 around the frequency $0.56(c/a)$. This suggests that the localized waveguide resonance in each hole can also result in enhanced transmission.

Similar behavior can also be expected in the optical regime for a real metal. Here we also calculate the normalized transmission through Au films with periodic array of the aperture by the 3D FDTD method. The Au film with a thickness of 200 nm is assumed to be on a glass substrate ($\epsilon = 2.117$), as considered in Ref. [8]. The time-domain auxiliary differential equation (ADE) approach is used to implement FDTD models of dispersive materials [17], where the discretization grid is 5 nm, and shows the convergence in our calculation. The dimensions of the holes are fixed at 225×75 nm^2 and the normalized transmission through the Au films with periodic aperture arrays for the different lattice constant $d = 425, 450, 475$ nm are calculated and shown in Fig. 4. The frequency-dependent permittivities of Au are referred to the literature [18]. For $d = 425$ nm, our result agrees well with the Fourier modal method calculation result in Ref. [8] [cf. the dashed lines in Fig. (3) of Ref. [8]]. The localized waveguide resonance corresponds to the peaks in the normalized transmission at the wavelength $\lambda = 836$ nm, i.e., the frequency $0.508(c/a)$ when $a = 425$ nm, and it hardly moves with differing lattice constants. It has been shown that for the real metal in the optics regime, the cutoff wavelength of metallic waveguides is increased significantly, and is much larger than Rayleigh's criterion for the PEC metallic waveguide [19,20]. Therefore, the cutoff wavelength for the 225×75 nm^2 aperture in the Au film is much larger

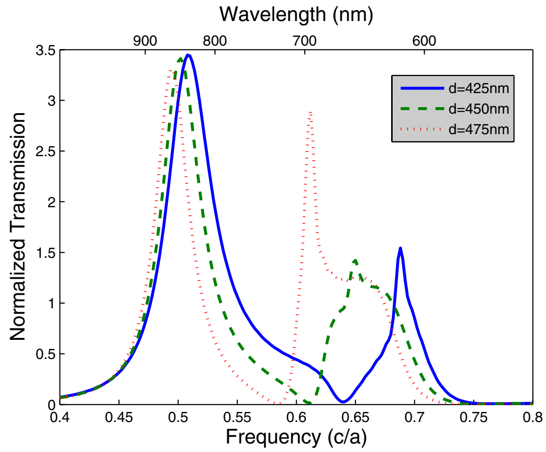


FIG. 4 (color online). The normalized transmission through the Au films with periodic aperture arrays for the different lattice constant $d = 425, 450, 475$ nm. The Au film is on a glass substrate ($\epsilon = 2.117$), the dimension of the hole is fixed at (225×75 nm^2), and the thickness of the films is 200 nm. The up (down) horizontal axis is labeled as the wavelength (frequency), where a is 425 nm.

than 450 nm. Since the transmission peak about the wavelength $\lambda = 836$ nm is almost independent of the lattice constant, we believe that the resonance is the localized waveguide resonance where each air hole is considered to be a section of metallic waveguide with both ends open to free space, forming a low-quality-factor resonator. This is also confirmed by our band structure calculations (not shown here) which give a flat band near the frequency $0.508(c/a)$. On the other hand, the position of the other transmission peak due to the surface plasmon depends on the lattice constant, which can be given approximately by the surface plasmon dispersion for a smooth film [6],

$$\lambda_{\max} = \frac{d}{\sqrt{i^2 + j^2}} \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}}, \tag{3}$$

where the integer index $\{(i, j)|i^2 + j^2 \geq 1\}$ is corresponding to the different set of peaks, ε_1 and ε_2 is the dielectric constant of the substrate and the metal, respectively. In Fig. 4, ($i = 1$, $j = 0$) corresponds to the peaks of the transmission at 617, 653, and 694 nm for the different lattice constant.

In conclusion, we have studied two different resonances, which contribute to the enhanced transmission through the metal films with periodic arrays of subwavelength holes: (i) the localized waveguide resonance (each air hole can be considered as a truncated rectangular waveguide with four metal walls and two sides open to air, and forms a low-quality-factor resonator), which is dependent on the holes shape but almost independent of the period of the structure; (ii) the property of the surface plasmon resonance due to the periodicity, which is directly connected with the lattice constant. The band structures of the resonant states are used to characterize the two different resonance. Both resonances play equally important roles in the enhanced transmission phenomena.

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