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Origin of superenhanced light transmission through two-dimensional subwavelength rectangular hole arrays

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Abstract. Superenhanced light transmission through subwavelength rectangular hole arrays have been reported and some investigations have been made into the physical origin of this phenomenon [K.J. Klein Koerkamp et al., Phys. Rev. Lett. **92**, 183901 (2004)]. In our current work, by performing FDTD (finite difference in the time domain) numerical simulations, we demonstrate that mechanism that is different from surface plasmon polaritons set up by the periodicity at the in-plane metal surfaces may account for this superenhanced light transmission. We suggest that for arrays of rectangular holes with small enough width in comparison to the wavelength of the incident light, standing electromagnetic fields can be set up inside the cavity by the surface plasmons on the hole walls with its intensity being substantially enhanced inside the cavity. So resonant cavity-enhanced light transmission is predominant and responsible for its superenhanced light transmission. Rectangular holes behave as Fabry-Pérot resonance cavities except that the frequency of their fundamental modes is restricted by their TM cutoff frequency. However we believe that both localized surface plasmon modes and surface plasmon polaritons set up by the periodicity at the in-plane metal surfaces have their shares in extraordinary optical transmission of rectangular hole arrays especially when the width of the rectangular hole is not small enough and the metal film is not thick enough.

PACS. 78.20.Ci Optical constants (including refractive index, complex dielectric constant, absorption, reflection and transmission coefficients, emissivity) – 73.20.Mf Collective excitations (including excitons, polarons, plasmons and other charge-density excitations) – 42.79.Dj Gratings

1 Introduction

The extraordinary transmission of light through a metallic film perforated by an array of subwavelength holes was demonstrated experimentally by Ebbesen et al. [1]. This enhanced light transmission was attributed to a resonant excitation of surface plasmon polaritons (SPPs) set up by the periodicity of the array at the in-plane metal surfaces [1–4]. They said that, collective excitations of the electron density on a metal surface, i.e. SPPs, can be set up provided that there is a periodic structure on this metal surface. The interaction between the incident radiation and the in-plane SPPs accounts for this extraordinary transmission. The coupling between the front and back surfaces of the metal film is crucial. However, Fabry-Pérot-like behaviors in metallic gratings have been studied [5,7,8]. They demonstrated that standing electromagnetic fields are set up inside the cavity and the extraordinary transmission was attributed to the resonant cavity-enhanced light transmission. The theoretical analysis in those papers showed that if there is a nonzero component of electric field of the incident light which is normal to the wall of the cavity, if the film is thick enough, and if the width of the grating grooves is small enough in comparison to the wavelength of the incident light, the surface plasmons on the upper and lower walls of the grating grooves interact, and standing electromagnetic waves are set up in the grooves, leading to a series of resonance peaks of transmission. It should be mentioned that the calculations in reference [8] are based on perfect conductors. It is commonly accepted that a perfect conductor does not support any excitation of surface plasmon resonance. However, despite the details inside the cavity, the author pointed out that although the resonance peaks associated with individual slit is very low, a periodic array of such slits can have a very large magnitude of the corresponding peaks. That is to say a grating acts as an amplifier of those resonances.

Influence of hole shape on extraordinary transmission through both isolated subwavelength holes and periodic arrays of subwavelength holes have been studied experimentally and theoretically [9–11]. When the depth of an isolated hole is shallow enough, an unexpected enhanced peak appears in the transmission spectrum [10]. A broad increase in transmissivity of a rectangular hole array was

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reported with respect to that of circular hole array [9,11]. In these papers the extraordinary transmission was attributed to the existence of shape resonances. In our current work, we have performed some numerical simulations on both square hole arrays and rectangular hole arrays with FDTD (finite difference in the time domain) method and found that if the metal film is thick enough, and if the width of the rectangular hole is small enough in comparison to the wavelength of the incident light, the mechanism for the superenhanced transmission of a rectangular hole array is fundamentally different from that for a square hole array. We suppose that resonant cavity-enhanced light transmission is predominant for arrays of rectangular holes with small enough width and is responsible for their superenhanced light transmission.

2 Principle of the calculations

In our FDTD calculations, the computing space and time are both discretized. The computing scheme is an explicit "leap-frog" scheme proposed by Yee in 1966. We have two sorts of FDTD program codes. One is similar to that in reference [13] which is easy to calculate transmission spectra. The other is designed to calculate distributions of both **E** fields and **H** fields. Our FDTD program codes include perfectly matched layer (PML) technique to solve the parasitical reflections at either end of the computing space in the propagation direction. In directions perpendicular to the propagation, periodic boundary conditions are used so that infinite two-dimensional arrays can be easily calculated. We can introduce a semi-infinite substrate by introducing it into the PML absorbing layer. Our FDTD program codes have been verified by transfer matrix method in the calculations of one- and two-dimensional photonic crystals.

The metal conductance is dependent on the frequency of incident light. However, if we are only interested in a very narrow range of frequency, for the sake of simplicity, we can take the conductivity to be a constant. In fact, if we are not to fit the experimental data precisely, for Ag at wavelength ranging between 600 nm and 1200 nm, even the calculations based on constant conductivity are sufficient for us to study the underlying physics. The square hole array and the rectangular hole array that we have studied are sketched in Figure 1. The cell is a 600×600 nm^2 square, the square hole is a 220×220 nm^2 square and the rectangular hole is a 60×400 nm^2 rectangle. In our calculation, the spatial mesh steps were set to $\Delta x = \Delta y = \Delta z = 10$ nm. The incident light is normal to the metal film with its **E** field perpendicular to the length of the rectangular hole. For metal we use a complex conductivity. It can be described by Drude model: $\sigma(\omega) = \varepsilon_r \varepsilon_0 \omega_p^2/(1/\tau - i\omega)$, where ω_p is plasma frequency, τ is relaxation time, and i is defined by $i^2 = -1$. We determine σ with these parameters of silver: $\omega_p = 1.374 \times 10^{16}$ rad/s and $1/\tau = 3.21 \times 10^{13}$ Hz [14]. In our calculations we use a σ at wavelength 600 nm, i.e. $\sigma = 5.9 \times 10^3 + 5.5 \times 10^5 i \quad (\Omega\text{m})^{-1}$.

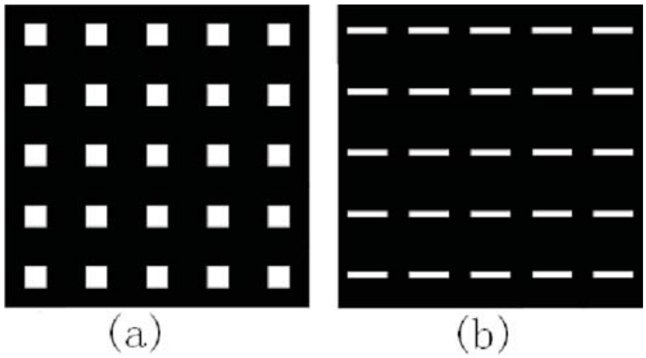

Fig. 1. Arrays of square holes (a) and rectangular holes (b).

3 Results and discussion

The in-plane SPPs and their role in the enhanced light transmission through a periodic array of subwavelength holes in a metal film have been studied experimentally and theoretically [1–4]. At normal incidence the peak positions of the enhanced light transmission are determined by [2]

$$\sqrt{i^2 + j^2}\lambda = a_0 \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}}$$

where i, j are integers; λ is the wavelength of incident light; a_0 is the period of the array and ε_1, ε_2 are dielectric constants of metal and interface medium respectively. From this equation we can see that if the dielectric constants of the front and back interface media are different, their corresponding peaks of the enhanced transmission do not overlap so that the coupling between the front and back surfaces is less effective. As a result, the intensity of the extraordinary transmission dramatically decreases. Thus if the in-plane SPPs are responsible for the extraordinary transmission, we can expect that the extraordinary transmission of a free-standing metal film is much larger than that with a substrate. However that is not the case if optically resonant cavity-enhanced light transmission is dominant. In this case the transmission associated with these cavity resonances is not very sensitive to the refraction index of the substrate [6].

Our numerical simulations seemingly indicate that for arrays of long and narrow rectangular holes resonant cavity-enhanced light transmission is dominant while for square hole arrays the in-plane SPPs set up by the periodicity and the coupling between the front and back surfaces are responsible for the enhanced light transmission. Figure 2 shows the enhanced transmissions through square arrays of square holes (a) and rectangular holes (b). Solid curves are for freestanding films and dotted curves for arrays on semi-infinite substrates with dielectric constant 2.0. Since the thicknesses of substrates are infinite (we realize it by introducing the substrates into PML absorbing layers), the curves may be slightly different from previous experimental or theoretical ones. It is evident that when a substrate is introduced, the transmissivity of a square hole array becomes very small while there is still a significant

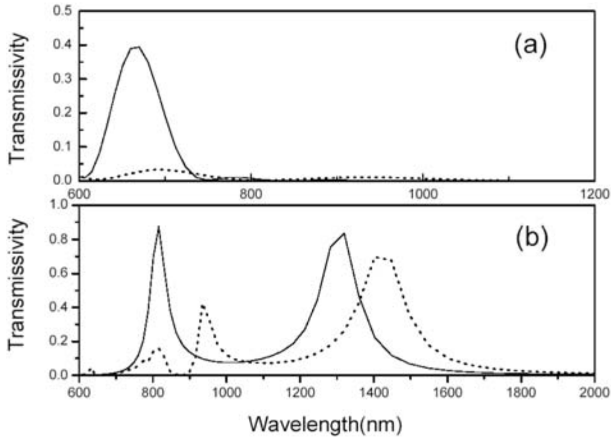

Fig. 2. (a) Numerically simulated enhanced transmission spectra of square arrays of 220 × 220 nm^2 square holes. Solid line is for a freestanding film and a semi-infinite substrate is introduced for dotted line with dielectric constant 2.0. (b) Numerically simulated superenhanced transmission spectra of 60 × 400 nm^2 rectangular hole arrays. Solid line is for a freestanding film and a semi-infinite substrate is introduced for dotted line with dielectric constant 2.0. For both (a) and (b) the cell is a 600 × 600 nm^2 square and the thickness is 300 nm.

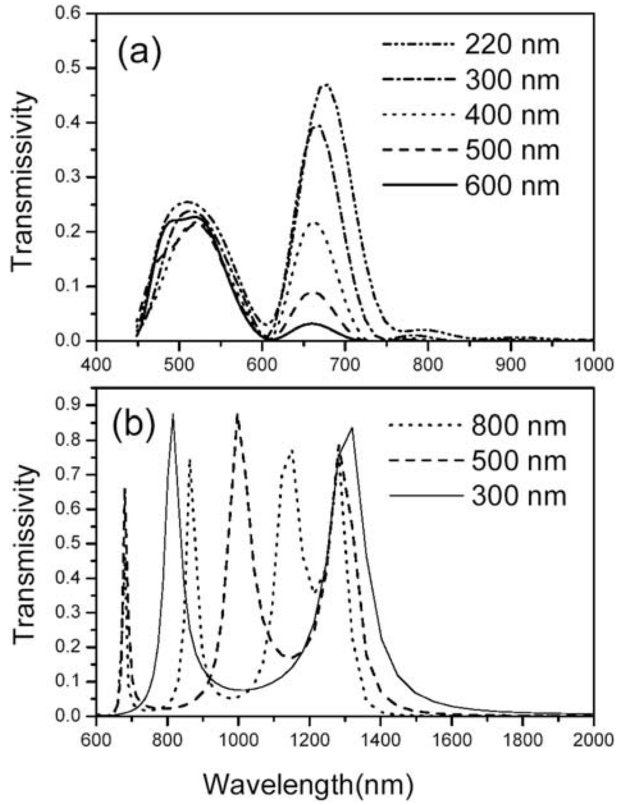

Fig. 3. (a) Numerically simulated enhanced transmission spectra of freestanding square arrays of 220 × 220 nm^2 square holes. The thicknesses of the films are 220 nm 300 nm, 400 nm, 500 nm and 600 nm. (b) Numerically simulated superenhanced transmission spectra of freestanding square arrays of 60 × 400 nm^2 rectangular holes. The thicknesses of the films are 300 nm (solid line), 500 nm (dashed line) and 800 nm (dotted line).

transmission for rectangular hole array in the range of so-called extraordinary transmission. This indicates different mechanisms for extraordinary transmission of arrays of different subwavelength features. Since the extraordinary transmission through rectangular hole array is not very sensitive to the permittivity of substrate, resonance inside the cavity may play an overwhelmed role in the extraordinary transmission. And according to our discussion above, suppression of extraordinary transmission by a substrate implies the excitation of in-plane SPPs and the coupling between the front and back surfaces that account for the extraordinary transmission of the square hole array.

The effect of the aperture depth on enhanced light transmission through square arrays of subwavelength cylindrical holes has been studied experimentally [12]. The in-plane SPPs set up by the periodicity were suggested to account for the extraordinary transmission. They pointed out that in the case of shallow holes, SPPs on the front and back surfaces couple via evanescent waves leading to enhanced light transmission. For deeper holes, the in-plane SPPs on the two surfaces can not couple and the transmission falls exponentially with the film thickness. However, for a grating consisting of narrow slits of infinite length, standing waves can be set up inside the cavity by the surface plasmons on the cavity walls and the intensity of zero-order maxima is always very large even when the thickness of metal film is very large. Figure 3 shows the enhanced transmission spectra through freestanding metal films of different thickness: (a) for square hole arrays and (b) for rectangular hole arrays. In (a) the thickness varies from 220 nm to 600 nm and in (b) the thicknesses are 300 nm (solid line), 500 nm (dashed line) and 800 nm (dotted line). It is clear that in (a), when the film becomes thicker, the peak falls very rapidly. This is qualitatively consistent with the experimental results reported by A. Degiron et al. [12], indicating that the in-plane SPPs and the coupling between front and back surfaces via evanescent modes are responsible for the enhanced light transmission. However, in (b), when the thickness increases, the peaks fall much more slowly than those in (a). When the thickness of the film is 300 nm, there is actually two peaks in the wavelength range larger than the period of the array. When the film becomes thicker, the third peak appears and when the thickness reaches 800 nm, the fourth one appears and so on. This phenomenon can be explained by that it is optical resonances inside the cavity instead of in-plane SPPs that accounts for the extraordinary transmission through a rectangular hole array. A peak appears whenever the cavity contains an integral number of half-wavelengths of the fundamental mode supported by the cavity, which is expressed by the Fabry-Pérot resonance condition: $m\lambda/real(n_{eff}) = 2d$, where m is an integer and d is the thickness of the metal film [7]. As a result of resonance, when the thickness gets larger, all the peaks move to larger wavelength and finally merge into the first one whose frequency is the cutoff frequency of TM mode of the cavity. However we could expect that if the film is too thin for a standing wave to exist inside the cavity, the mechanism for the extraordinary transmission will fundamentally change. In-plane SPPs, localized surface plasmon modes and the coupling between the front and back surfaces will be predominant. A slit of definite length has a cutoff frequency of TM mode. The immovability of the first peak is due to its TM cutoff frequency. Modes with frequency lower than this cutoff frequency will be forbidden.

Because the dispersion properties of light waves and surface plasmon waves are different, generally the incident light can not couple to surface plasmons on the metal surface. However, a periodic structure will set up SPPs and enable the coupling between the incident light and the surface plasmon waves. If the enhanced light transmission is due to a resonant excitation of in-plane SPPs set up by the periodicity, the positions of the enhanced transmission peaks scale exactly with the lattice constant of the periodic structure, independent of geometrical parameters of the aperture and film thickness [1]. Our calculations showed that the enhanced transmission of rectangular hole arrays does not scale with the periodicity. Figure 4 shows the extraordinary transmission of square arrays of square holes (a) and rectangular holes (b). The thickness is 400 nm and periods are different: dashed line for period 600 nm and solid line for period 800 nm. In (a) the holes are 300×300 nm^2 squares and in (b) the holes are 60×400 nm^2 rectangles. It is evident that in (a) the extraordinary transmission peaks scale exactly with the periodicity while in (b), the two curves have nearly the same peak positions regardless of their different periods. So the peak positions of rectangular hole arrays may be determined mainly by the geometrical parameters of the cavity. This is sufficient for us to conclude that for an array of rectangular holes with small enough width, the resonant cavity-enhanced light transmission is dominant. However, transmission spectra of rectangular hole arrays as a function of period have been studied experimentally [11]. Shifts of peak positions and variations of peak intensities with period was reported. Although the rectangular hole arrays they studied may support propagating modes in so-called extraordinary transmission range, the width of the rectangular hole is too large to achieve substantial enhancement of **E** field inside the cavity. If the width is small enough, the power of incident light will be collected into the cavity and the transmission peaks no longer scale with the period. Note that the normalized transmission peak of the dashed curve in Figure 2 of reference [9] (width 75 nm for wavelength 900 nm) is much higher than that of solid line in Figure 3 of reference [11] (width 200 nm for wavelength 600 nm).

The modes inside a square waveguide are fundamentally different from those inside a slit of infinite length and standing waves of Fabry-Pérot-like modes generally exist in a slit. However we suppose that a slit of definite length will support the resonant peak with frequency larger than the cutoff frequency of TM mode(its magnetic field parallel to the slit). A rectangular hole can be regarded as a slit of definite length that supports standing waves of Fabry-Pérot-like modes with its **E** fields being substantially enhanced inside the cavity provided that its width is small enough in comparison to the wavelength of incident light. Thus the resonant peaks of Fabry-Pérot-like modes can be expected to occur inside this definite slit with frequency larger than the TM cutoff frequency and those with frequency smaller than the TM cutoff frequency will be forbidden. The TM cutoff frequency of a rectangular hole is smaller than that of an equivalent square hole. And as has been stated in reference [7], for a real metal, finite conductance have a strong effect on the fundamental modes inside the cavity and further enlarge the TM cutoff wavelength due to the skin effect. So the rectangular cavity made of real metal may support propagating modes in so-called extraordinary transmission range. We can consider a Fabry-Pérot-like mode as a combination of a series of backward and forward propagating eigenmodes inside the cavity. So propagating modes inside the rectangular cavity are channels of standing waves of Fabry-Pérot-like modes that account for the superenhanced transmission through a rectangular hole array while enhanced transmission through a square hole array is due to evanescent modes.

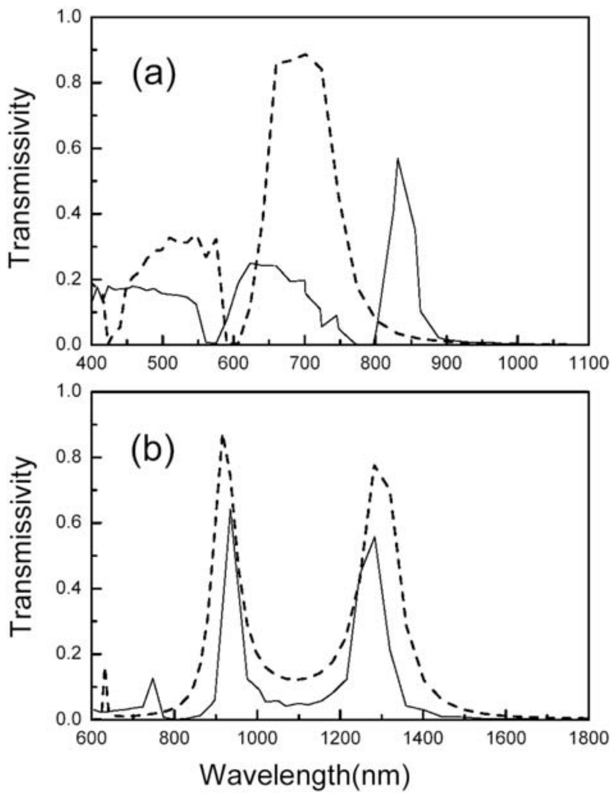

Fig. 4. Numerically simulated transmission spectra of freestanding square arrays of (a) the same 300×300 nm^2 square holes and (b) the same 60×400 nm^2 rectangular holes but the periods of the arrays are different. The period of the dashed curves is 600 nm and that of the solid curves is 800 nm. For both (a) and (b) the thickness is 400 nm.

In order to gain further insight into the underlying physics of superenhanced light transmission of rectangular

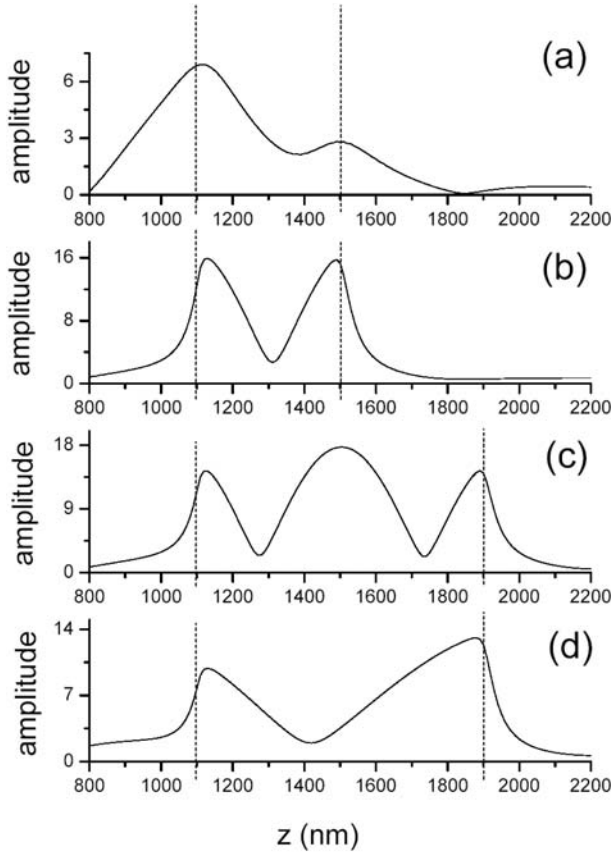

Fig. 5. Numerically simulated distributions of amplitudes of **E** fields at the center of the rectangular holes. Between the two vertical lines are the metal films, (a) is for the peak in Figure 3a with thickness 400 nm and wavelength 670 nm, (b) corresponds to the peak in Figure 4b (solid curve) with wavelength 920 nm, (c) is for the peak in Figure 3b with thickness 800 nm and wavelength 850 nm and (d) for the peak of this curve with wavelength 1280 nm.

hole arrays, the distributions of amplitude (i.e. modulus) of **E** fields at the center of the rectangle are numerically simulated along z axis by FDTD method. The results are shown in Figure 5. Between the two vertical dashed lines are metal films. (a) is for the peak in Figure 3a with thickness 400 nm and wavelength 670 nm. It is clear that for a square hole array, the modes inside the square hole are evanescent. The **E** fields are significantly enhanced near the two interfaces, indicating an excitation of in-plane SPPs. (b) corresponds to the peak in Figure 4b (solid curve) with wavelength 920 nm. (c) is for the peak in Figure 3b with thickness 800 nm and wavelength 850 nm and (d) for the peak of this curve with wavelength 1280 nm. It is evident that in (b), (c) and (d), standing waves are established inside the cavity. These modes do not decay in the z direction. In (b), there is one node inside the cavity and in (c), there are two nodes. Note that in (b), (c) and (d), **E** fields are rather weak outside the cavities and are substantially enhanced inside the cavities. This implies that instead of the excitation of in-plane SPPs, cavity-enhanced light transmission is dominant. It seems that there is one node in (d). However, this peak can not move with thickness to satisfy Fabry-Pérot resonance condition. Generally the structure of its electromagnetic fields is rather complicated. Note that the modes inside the cavity are propagating and in some specific condition it is possible to establish standing waves inside the cavity at the wavelength of this peak

4 Summary

We have performed some FDTD numerical simulations of extraordinary light transmission of both square hole arrays and rectangular hole arrays. We found a superenhanced light transmission for rectangular hole arrays with respect to the square hole arrays even though the hole size actually decreases. This is qualitatively consistent with the results in reference [9,11]. We found that if the film is thick enough and the width of the rectangular hole is small enough in comparison to the wavelength of incident light, the mechanism for its superenhanced light transmission is fundamentally different from that of square hole array. For arrays of rectangular holes with small enough width, we propose that a constructive interference of Fabry-Pérot-like resonances localized in each cavity is responsible for its superenhanced light transmission. However we believe that both localized surface plasmon modes and in-plane SPPs set up by the periodicity have their shares in extraordinary optical transmission through rectangular hole arrays especially when the width of the rectangular hole is not small enough and the film is not thick enough.

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