

# Effect of nanoholes on the plasmonic properties of star nanostructures

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## ABSTRACT

The transmission and localized electric field distribution of nanostructures are the most important parameters in the plasmonic field for nano-optics and nanobiosensors. In this paper, we propose a novel nanostructure which may be used for nanobiosensor applications. The effect of nanoholes on the plasmonic properties of star nanostructure was studied via numerical simulation, using the finite-difference time-domain (FDTD) method. In the model, the material type and size of the nanostructures was fixed, but the distance between the monitor and the surface of the nanoholes was varied. For example, nanoholes were located in the center of the nanostructures. The simulation method was as follows. Initially, the wavelength of incident light was varied from 400 to 1200 nm and the transmission spectrum and the electric field distribution were simulated. Then at the resonance wavelength (wavelength where the transmission spectrum has a minimum), the localized electric field distribution was calculated at different distances from the surface of the nanostructures. This study shows that the position of nanoholes has a significant effect on the transmission and localized electric field distribution of star nanostructures. The condition for achieving the maximum localized electric field distribution can be used in nano-optics and nanobiosensors in the future.

**Keywords:** Nanoholes, plasmonic, optical properties, nanostar

## 1. INTRODUCTION

Metal nanoparticles (NPs) play an important role in nanotechnology and optical fields that break through the diffraction limit [1]. The coherent oscillations of conduction-band electrons of noble metals, such as gold and silver, are generally termed plasmons [2]. Recently, the science and technologies that focus on optical properties of metal nanostructures have grown into an independent research field known as "plasmonics"[3]. Nanoparticles can 'focus' light into the nanometer scale and provide near-field optical microscopy with higher resolution than the previous traditional optical methods [4]. Many researcher are interested in the modeling and simulation of the optical properties of complex nanostructures, because the simulation results can provide a detailed, quantitative understanding of these optical systems. These advances have interplayed between theory and experiment, which has enable the design of optimized plasmonic nanostructures to guide the experimental procedures. The transmission and localized electric field distribution are the most important parameters in the plasmonic field for nano-optics and nanobiosensors. We have the simulation of the optical properties of complex nanostructures [5-7].

In this paper, we propose complex nanostructures which may be used for nanobiosensor applications in the future. The plasmonic properties of complex nanostructures were studied via numerical simulation using the finite-difference time-domain (FDTD) method. The fundamentals of the FDTD method are to solve Maxwell's Curl equations in the time domain after replacement of the derivatives by finite differences [8, 9]. It has been applied to many problems of propagation, radiation and scattering of electromagnetic waves [10]. Plasmonic effects of nanoparticles are relevant to the enhanced local electromagnetic fields near the surfaces of nanoparticles. Smooth surfaces do not result in significant enhancement, while sharp nanostructures or nanoholes can result in the enhancement of the localized surface plasmon resonance (LSPR). Nano-pentagrams have more sharp structures than the traditional triangle nanostructures, which is the merit of polygons for achieving enhanced transmission and electric field distribution. Therefore, it is very important to

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explore the effect of nanoholes on the plasmonic properties of star. The model of our designed nanostructures, simulation results and discussions are introduced in the followed paper.

## 2. COMPUTATIONAL SETUP

Plasmonic properties of pentagrams with and without nanoholes were derived. We optimized the design by selecting material parameters (refractive index, extinction coefficient, permittivity, and permeability, wavelength of incident light, dimension and shape of the nanoholes). Design and simulation of the nanoholes was performed using commercially available software, three-dimensional FDTD Solution. The FDTD has computational advantages of reducing memory requirements and ease in treating complex materials and shapes. Figure 1 shows our designed geometrical model of the Ag pentagram nanostructures. The pentagram nanostructures were oriented in the  $x$ - $y$  plane and the incident light polarized in the  $x$ -axis propagates along  $z$  axis. The out-of plane height of the Ag nanostructures was 40 nm. The in-plane widths of nanostructures was 500 nm. The in-plane widths of nanoholes was 250 nm and the refractive index of the medium surrounding the Ag nanostructures was 1.0 (air). For the Ag material, we used the Drude model [11,12] to calculate the transmission and localized electronic distribution near the surface of the pentagram nanostructures.

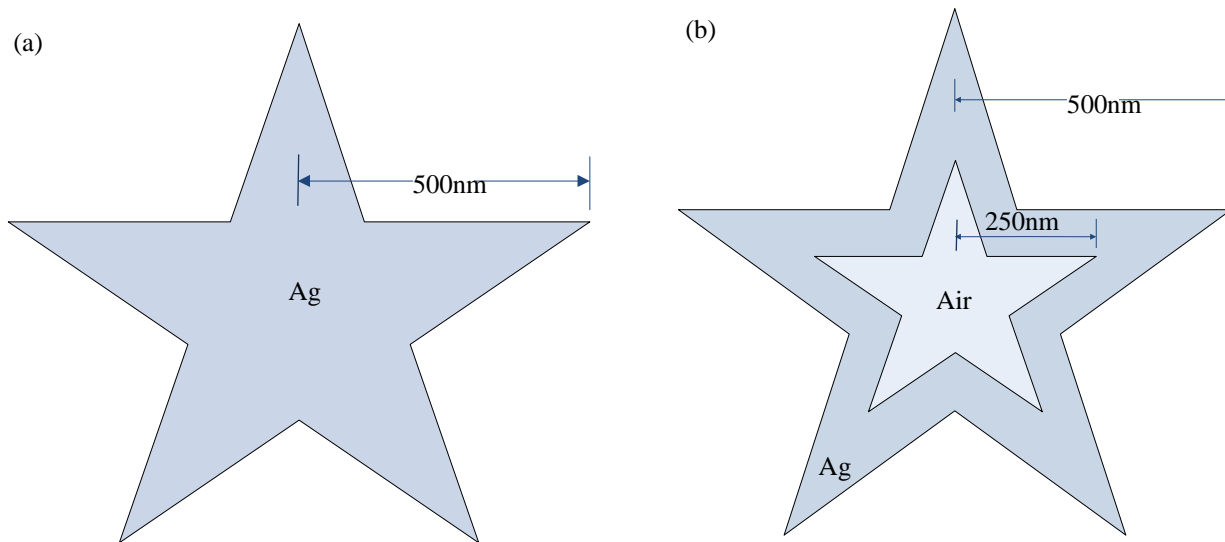


Figure 1. Designed geometrical model of Ag pentagram nanostructures. (a) Pentagram nanostructure without nanohole; (b) Pentagram nanostructure with air nanohole

## 3. COMPUTATIONAL RESULTS AND DISCUSSION

### 3.1 Transmission results

According to the design model shown in Figure 1, we simulated the transmission in the  $z$  direction and localized electric field distribution near the surface of the nanostructures using the FDTD method. The simulation parameters of the FDTD algorithm were set as follows: the incident light ranges from 400 nm to 1200 nm with plane wave in the normal incidence angle  $\theta = 0^\circ$ . The distance between the surface of the nanostructures and the monitor for transmission is 920 nm. The distance between the light source and the surface of the nanostructures is 940 nm. The meshing size in the  $x$  and  $y$  planes (two-dimensional simulation) was,  $\Delta x = 2$  nm and  $\Delta y = 2$  nm, respectively. Simulation time,  $t$ , (theoretically,  $t = \Delta x/2c$ ,  $c$  is the velocity of light) was set to be 125 fs. The output results are the relationship between the transmission and the incident wavelength. Figure 2 (a) gives the transmission of the pentagram nanostructure calculated by the FDTD method. Figure 2 (b) is the transmission of nanostructure with nanohole. From Figure 2, we can see that the minimum values of the transmission are 520 nm, and 550 nm. They correspond to the plasmonic resonance wavelengths. The shapes of the transmission are similar, because the transmission is the far field effect for the nanostructures. The peak of transmission is 0.95 which is close to the maximum transmission in the traditional optical field.

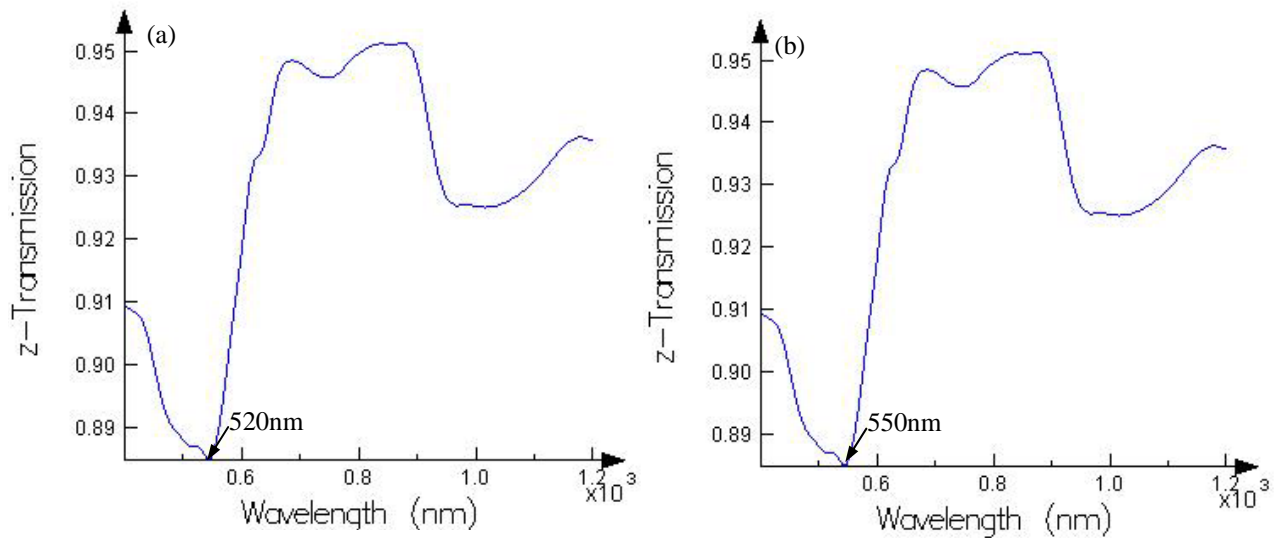
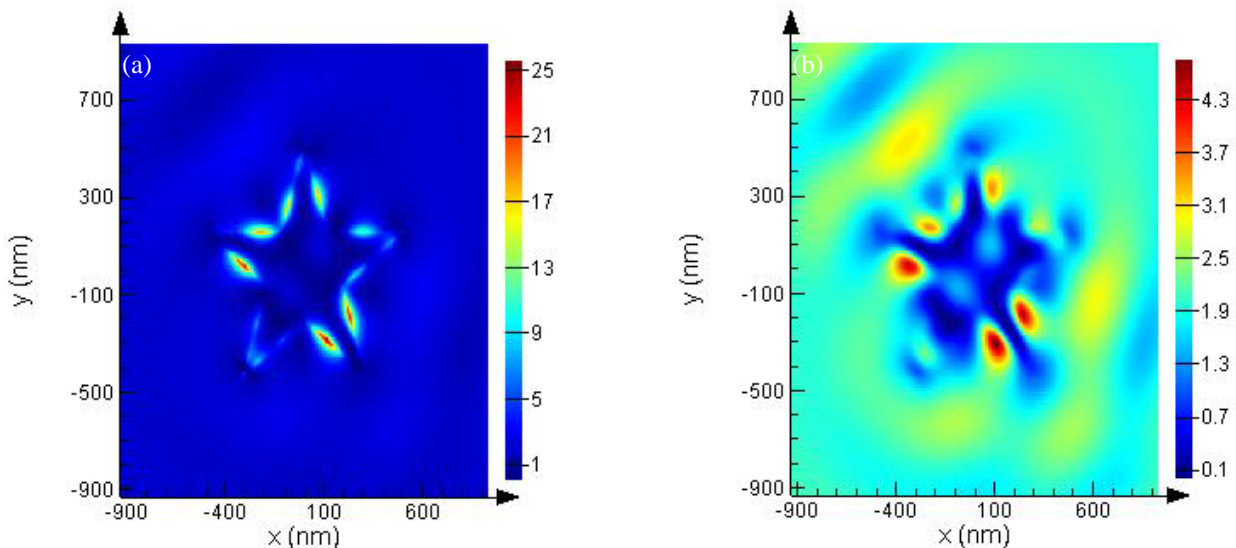


Figure 2. The transmission of the pentagram nanostructures calculated by FDTD. (a) without nanohole; (b) with nanohole

### 3.2 Near field electric intensity distribution for the nanostructures without nanoholes

In order to fully understand the optical response of our designed nanostructures, we carried out the numerical simulation of electric field ( $E$ -field) intensity distribution from the surface of the nanostructures in the near field boundary.  $E$ -field distributions in the  $x$ - $y$  plane at various distances from the surface of the nanostructures are shown in Figures 3 (a), 3 (b), 3 (c), 3 (d) and 3 (e), respectively. The incident wavelength is 520 nm, just as the resonance wavelength of the nanostructures. The distances between the monitor and the surface of the nanostructures are 20 nm (Fig. 3 (a)), 60 nm (Fig. 3 (b)), 100 nm (Fig. 3 (c)), 140 nm (Fig. 3 (d)) and 180 nm (Fig. 3 (e)). From Figure 3, we can see that there is a significant field enhancement at the metal-air interface in the regions between the sharps structures. The  $E$ -field distribution is asymmetric because of the illumination which was TM linear polarized. The maximum  $E$ -field intensity varies with distance. There are no effects of the nanostructures for  $E$ -field distribution when the monitor is far away from the surface of the nanostructures. The maximum value of the  $E$ -field intensity is 25 when the distance is 20 nm, while it reduces to 2.9 when the distance is more than 100 nm. Therefore, the effective distance of plasmonic enhancement produced by the nanostructures is about 100 nm.



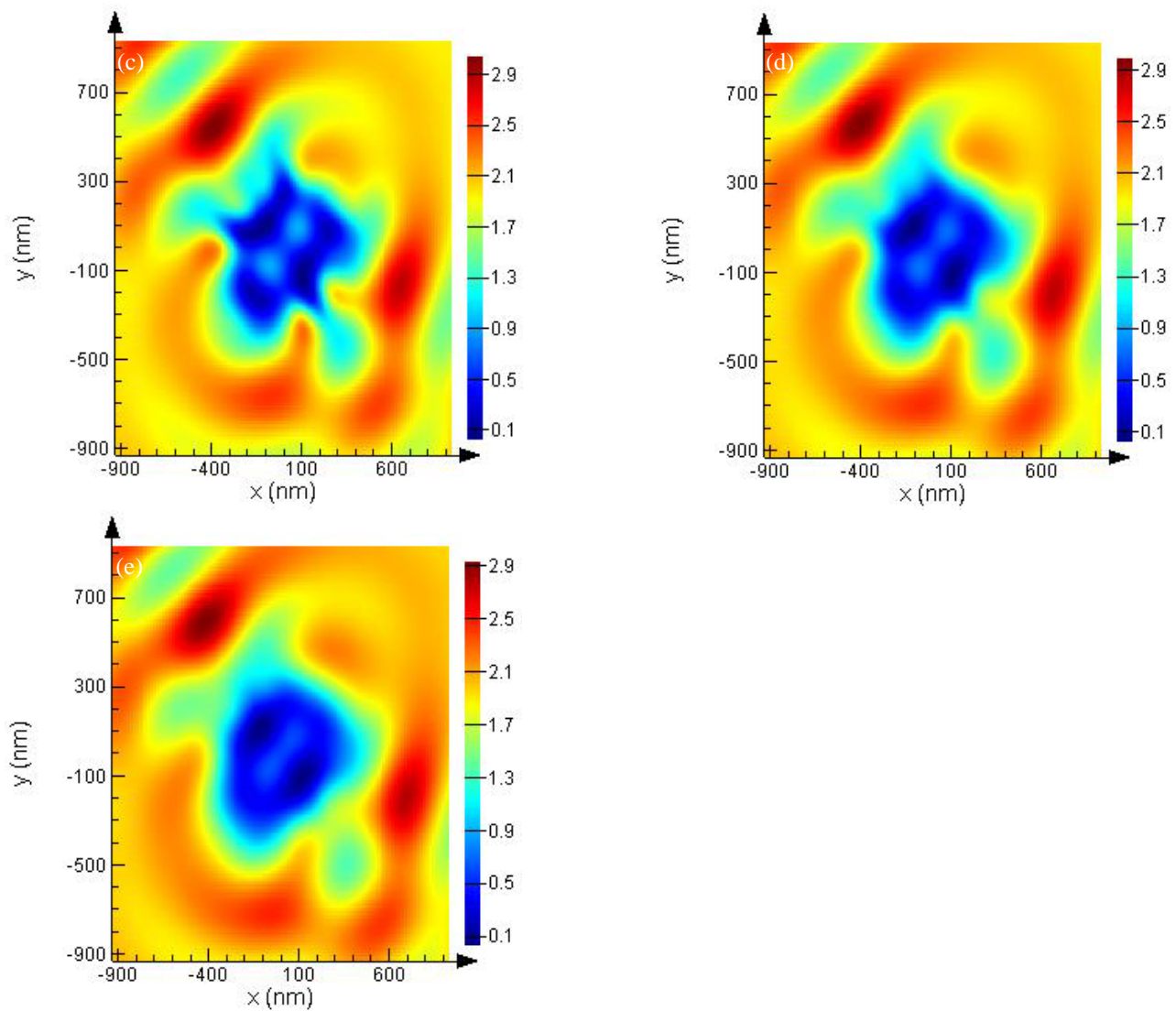
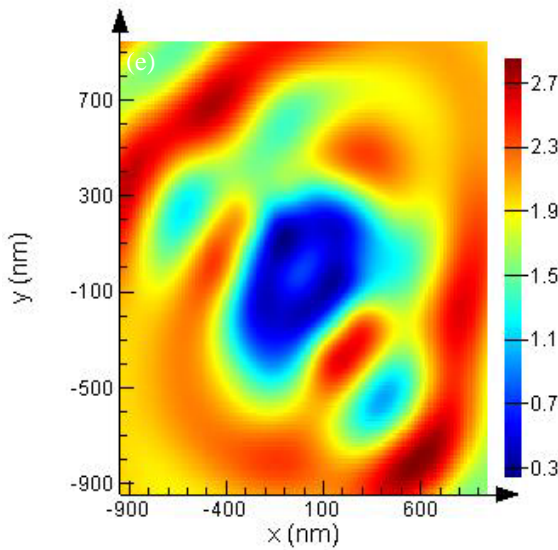
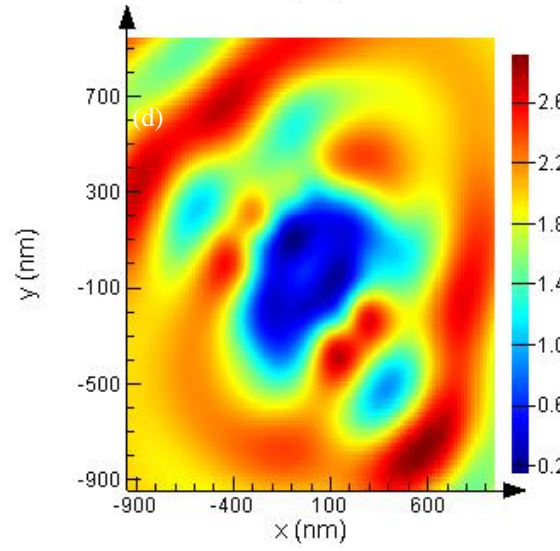
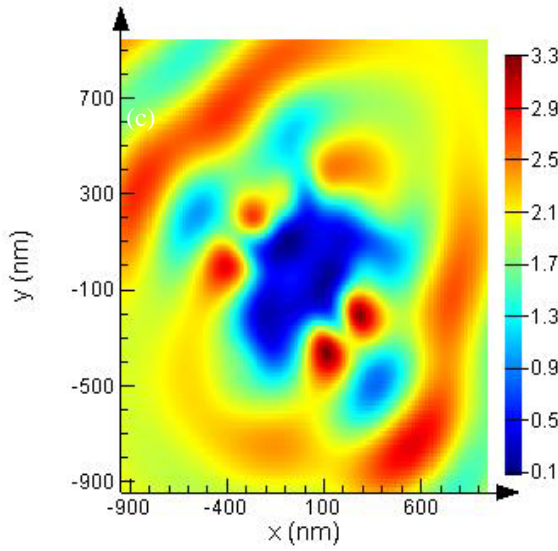
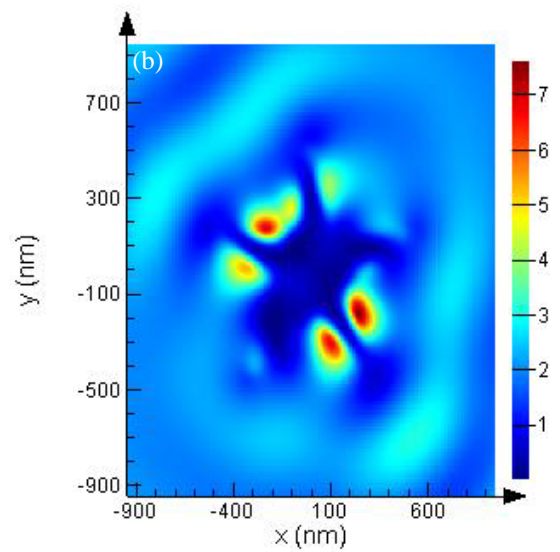
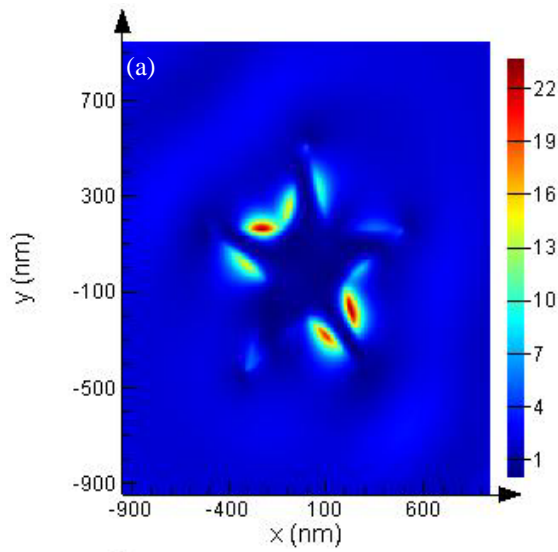


Figure 3. Near field electric intensity distribution in the transmission direction of the Ag pentagram nanostructures calculated by FDTD when the distances between the monitor and the surface of the nanostructures are (a) 20 nm; (b) 60 nm; (c) 100 nm; (d) 140 nm; (e) 180 nm.

### 3.3 Near field electric intensity distribution for the nanostructures with nanoholes

The  $E$ -field intensity distributions in the  $x$ - $y$  plane for various distances from the surface of the nanostructures with nanoholes are shown in Figure 4 (a), 4 (b), 4 (c), 4 (d) and 4 (e), respectively. The resonance wavelength of the nanostructures at 550 nm was selected as the incident wavelength. The distances between the monitor and the surface of the nanostructures are the same as Figure. 3. From Figure 4, we can see that the maximum  $E$ -field intensity is 22 when the distance between the monitor and the surface of the nanostructures with nanoholes is 20nm. There are obviously enhancements in  $E$ -field intensity when the distances are 20 nm and 60 nm. Comparing the results of Figures 3 and 4, we found that nanoholes have a strong effect on the electric field distribution in the near field domain, especially at a distance of 100 nm. The electric field intensity and distribution are similar for a distance of 20 nm, for the nanostructure with and without holes. This was also true when the distance was increased to 60 nm. When the distances are larger than 100 nm, the distribution maps are different for the two different nanostructures, while the intensities remain similar. The nanoholes did not any effect on the  $E$ -field intensity when the distances are larger than 180 nm. The nanostructures with or without nanoholes have the same distribution.



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## 4. CONCLUSION

In summary, we focused on the effect of nanoholes on the plasmonic properties of pentagram nanostructures. The transmission and near field distribution were simulated by the FDTD method. The calculated results show that nanoholes have a strong effect on the distribution in the near field domain, especially at a distance of 100 nm. When the distances are larger than 100 nm, the distribution maps are different for the two structures, while the intensities remain similar. The nanoholes do not any effects on the E-field intensity when the distances are larger than 180 nm.

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