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LSPR spectral properties of Au nano-ring arrays and single Au nanoparticles

MA Jun-xian, TAN Rui-hu, FANG Yu, ZHENG Da-wei, LUO Xian-gang

(*Advanced Technology Research Center, Shenzhen University, Shenzhen* 518060, *China*)

Abstract: In this paper, we simulate Localized Surface Plasmon Resonance(LSPR) absorption of periodic Au nano-ring arrays and single Au nanoparticles using the Finite Difference Time Domain(FDTD) method. We choose input plane waves of different wavelengths and discuss the relation between the absorption peak of the Au array and the variable external dielectric constants. It is found that the sensitivity of these sensors based on LSPR is improved compared to the common sensors and the enhancement is caused by the periodical structure. We also investigate the spectrum characteristic of a single Au nanoparticle and discuss the relation between the absorption peak and the size of the nanoparticle.

Key words: LSPR; absorption spectrum; 3D FDTD; nanoparticles

1　Introduction

Localized Surface Plasmon Resonance (LSPR) accounts for intense dispersion and absorption when metal nanoparticles are incited by visible light or infrared ray. It is a physical phenomenon caused by the resonant coupling between the incident electromagnetic field and the conduction electrons in the metal. When the external dielectric constant is a constant, metal nanoparticles have an obvious absorption at a particular wavelength of the incident light and the surface plasmon wave is localized by the surrounding the metal nanoparticles. We analyze the LSPR spectral properties to study the LSPR phenomenon based on the metal nanostructure. When we change the dielectric constant, the absorption peak will shift. By using this optical characteristic, LSPR could be used in material sensors to achieve highly sensitivity. In this paper, we focus on the shifts of LSPR absorption peak when the dielectric constant and the size of metal nanoparticles are changed.

2　Numerical simulation and parameter setting

We choose the Lorentz-Drude model to analyse the LSPR phenomenon of the metal dispersion material, and the LSPR absorption peak is calculated from Maxwell equations using a 3D Finite Difference Time Domain(FDTD) simulation method.

The parameters of Au nano-ring array simulation are: TM plane wave; wavelength(1 220 – 2 600

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nm); 3 × 3 Au nano-ring array placed on the glass substrate; the height of Au ring is 40 nm with a thickness of 35 nm and the period is 400 nm. The parameters of a single Au nanoparticle simulation are: TM plane wave; wavelength (1 080 – 1 400 nm); a single Au nanoparticle placed on the glass substrate; height is 40 nm, and the radius is set to 150, 175, 200, 225, 250, 275 or 300 nm. The absorbing boundary condition is chosen to be a perfectly matched layer (PML) absorbing boundary condition for all the simulations.

3 Results and Conclusions

Fig. 1 shows the structure of the Au nano-rings array and its energy distribution at $\lambda = 1\,440$ nm, with the green parts in the right hand chart denoting high energy. From Fig. 1 we can see that the energy is centralized on the edges of particles, which means the energy absorption of the incident light is concentrated in the exterior of the Au nano-rings.

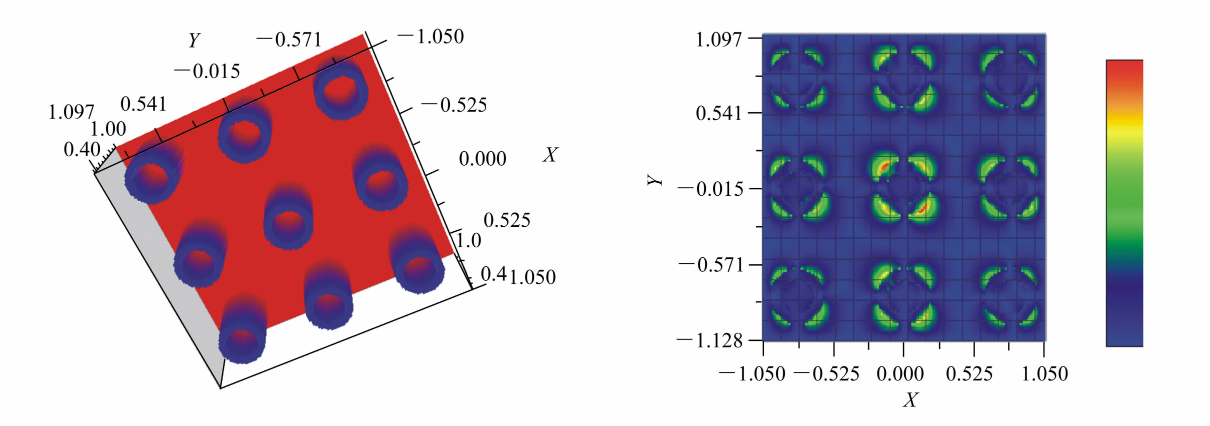

Fig. 1 Structure of the Au nano-ring array and its energy distribution at $\lambda = 1\,440$ nm.

In order to study the relationship between the dielectric constant and the absorption peak, we set $n = 1$, 1.3, 1.4 respectively, and the results are shown in Fig. 2. We can see the absorption peak locates at 1 500, 1 800, 1 900 nm, respectively, and the position of absorption peak is red-shifted when the dielectric constant is increasing. The peak is shifted about 100 nm while the dielectric constant increases by 0.1.

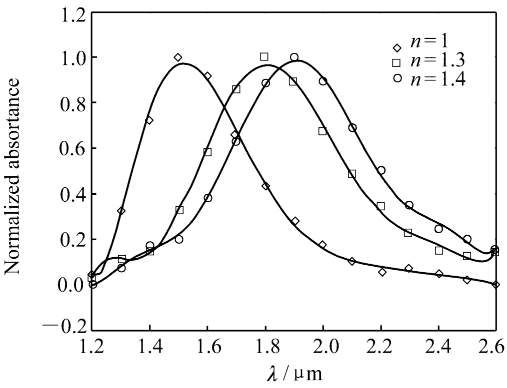

Fig. 2 Absorption spectrum of Au nano-rings.

Then we undertook a comparative experiment of a single Au nanoparticle and a 3 × 3 Au array to determine whether the period affects the absorption peak, and we used an Au nanoparticle with the same

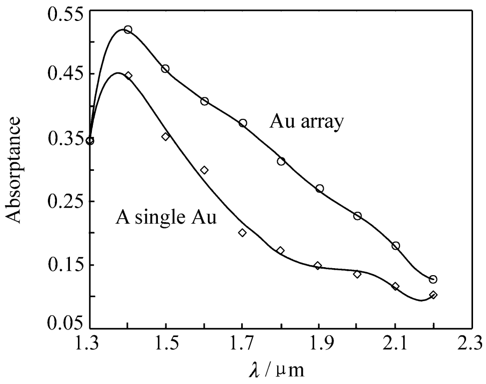

Fig. 3 Comparison of a single Au nanoparticle and 3 × 3 Au array.

radius and height. It was found that the period has little effect on the absorption peak position, but has a large affect on absorption intensity, as shown in Fig. 3. That means the periodical nano-structures can localize and enhance the electromagnetic field selectively, leading to a stronger absorption.

At last, we investigate LSPR spectral properties of a single Au nanoparticle and discuss the relationship between the absorption peak and the size of a single Au nanoparticle by performing 7 comparative experiments. We present the structure of single Au nanoporticle and its energy distribution in Fig. 4. We also found that the energy is centralized on the edges of particles as shown in Fig. 1.

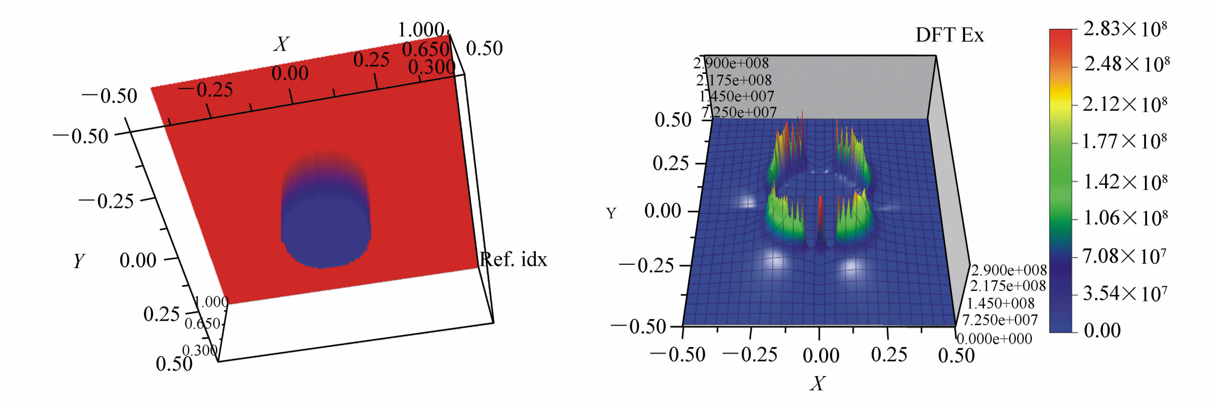

Fig. 4　Structure of single Au nanoparticle and its energy distribution at $\lambda = 1\ 380$ nm.

From the left chart in Fig. 5, we can see that the absorption peak is red-shifted when the radius of Au nanoparticle is increasing. The right picture shows a linear relationship between the radius and the location of absorption peak, and the wavelength of absorption peak increases when the radius is increasing. There are two inflection points between 150 nm and 175 nm and between 275 nm and 300 nm, respectively. Furthermore, we can see the slope between 150 nm and 175 nm is larger, which means the Au nanoparticle whose radius is smaller than 175 nm is more sensitive around the absorption peak.

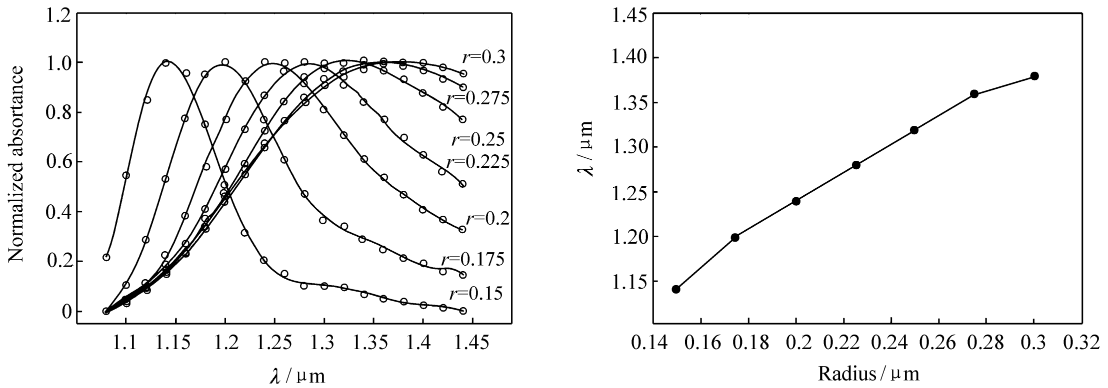

Fig. 5　Absorption spectrum of an Au nanoparticle of different sizes and the relationship between the radius of the Au nanoparticle and peak position.

3 Conclusions

From our simulation experiments, we can conclude that the absorption peak will shift when the dielectric constant is changed, and the intensity of absorption is related to the dimension of the single particle. The periodic nanostructure can localize and enhance the electromagnetic field selectively, therefore, its sensitivity can be improved by increasing the number of periodic particles. Furthermore, there is a linear relationship between the radius and the absorption peak, and the two inflection points. The result means that Au nano-particles are more sensitive to the change of wavelength when the radius is below a certain value, so we can control the position of the LSPR absorption peak by designing different sizes of metal nanoparticles.

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Author biography: Ma Jun-xian (1961—), male, professor of Advanced Technology Research Center of Shenzhen University, his research interests are subwavelength optical devices and broadband optical network, *etc.*
E-mail: majx@szu.edu.cn