Controlling optical properties of periodic gold nanoparticle arrays by changing the substrate, topologic shapes of nanoparticles, and polarization direction of incident light*

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The effects of various parameters including thickness and dielectric constants of substrates, shapes of nanoparticles, and polarization direction of incident light, on the extinction spectra of periodic gold nanoparticle arrays are investigated by the full-vectorial three-dimensional (3D) finite difference time domain (FDTD) method. The calculated results show that the substrate affects the extinction spectra by coupling the fields co-excited by the substrate and gold nanoparticles. Extinction spectra are influenced by the shapes of the nanoparticles, but there are no obvious changes in extinction spectra for similar shapes. The polarization direction of incident light has a great influence on the extinction spectra. The implications of these results are discussed.

Keywords: localized surface plasmon, extinction spectra, gold nanoparticles

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1. Introduction

Metal nanoparticles usually exhibit localized surface plasmon resonance (LSPR) caused by the collective oscillation of electrons upon light excitation.[1] The excitation of LSPR results in the occurrence of pronounced extinction band[2] and local field enhancement effects,[3] which have important applications in potential chemical or biological nanosensors.[4] Different applications require different LSPR properties. For an isolated metal spherical particle, the linear optical properties are well described by the Mie theory.[5] Two interacting gold nanoparticles can lead to additional resonances for the coupled system.[6] For muliti-nanoparticles, such as two-dimensional (2D) patterns of periodic metal nanoparticle arrays, many experimental investigations and theoretical calculations have shown that the characteristics of the resonance, such as central frequency, bandwidth, amplitude, and line shape, depend on the particle size,[7] shape,[8] surrounding medium,[9] lattice constant,[10] and the arrangement of the periodic metal nanoparticle arrays.[11] Therefore, it is possible within certain limits to design extinction spectra by controlling some specific parameters.

In this paper, we investigate the extinction spectra of the nanostructures composed of periodic gold nanoparticle arrays and dielectric substrate. Different thicknesses and dielectric constants of the substrate and different topologic shapes of gold nanoparticles are considered. Meanwhile, we study the influence of the nanostructures on extinction spectra by changing the polarization direction of incident light. Ten topologic shapes of gold nanoparticles, including diamond, circular ring, rectangular ring, pentagonal ring, five-pointed star, flower, L, Y, T, and X, are discussed. In our work, all the results are obtained by the full-vectorial three-dimensional (3D) FDTD method based on a square uniform mesh. The grid size is set at 2 nm and the permittivity function of gold can be well described by a Drude–Lorentz model. The parameters used in our simulations are determined by the experimental data of Johnson and Christy.[12]

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2. Effect of thickness and dielectric constant of the substrate

A sketch of periodic gold cylindrical nanoparticle arrays deposited on the substrate supported by quartz-glass is shown in Fig. 1. The radius and height of a single gold cylindrical nanoparticle are 50 nm and 100 nm, respectively. Gold nanoparticles of this size can be easily fabricated by electron beam lithography techniques. In our simulations, the X direction is the same direction as the source injection and absorbing boundaries are used in this direction. Six gold nanoparticles are arranged in a line along the X direction, which is enough for our simulations.[13] The lattice constant is kept at 450 nm. Periodic boundaries can be applied in the Y direction. The TE polarization of incident light is adopted in order to observe the extinction spectra effectively.

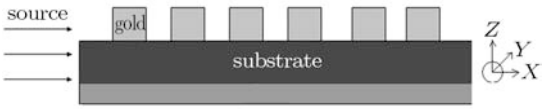


Fig. 1. Sketch of periodic gold nanoparticle arrays deposited on the substrate supported by quartz glass.

First, the influence of the substrate thickness on the extinction spectra is investigated. Indium tin oxide (ITO) films with thicknesses of 0, 20, and 140 nm are used as substrates, respectively. As shown in Fig. 2(a), the simulated extinction spectra appear to be different greatly from each other (Fig. 2(b)), revealing that the substrate thickness has a strong influence on the optical properties of the nanostructures. According to the optical waveguide theory,[14] the cut-off wavelength satisfies the following formula

$$\lambda_{\rm cut} = \frac{2\pi t\sqrt{\varepsilon_{\rm sub} - \varepsilon_{\rm glass}}}{m\pi + \arctan\left(\sqrt{\dfrac{\varepsilon_{\rm glass} - \varepsilon_{\rm air}}{\varepsilon_{\rm sub} - \varepsilon_{\rm glass}}}\right)}, \qquad (1)$$

where t is the substrate thickness, $\varepsilon_{\rm sub}$ ($\varepsilon_{\rm sub} = \varepsilon_{\rm ITO} = 3.61$), $\varepsilon_{\rm glass}$ ($\varepsilon_{\rm glass} = 2.28$), and $\varepsilon_{\rm air}$ ($\varepsilon_{\rm air} = 1$) are dielectric constants of the substrate, glass, and air, respectively. According to formula (1), when the wavelength of the incident light ranges from 500 nm to 900 nm, there is no waveguide mode in the substrate with a thickness of 20 nm, and there is TE_0 waveguide mode in that of 140 nm. The interactions of the fields caused by LSPR among gold nanoparticles can be ignored due to the large lattice constant. In the 0 nm thickness case, the extinction spectrum is mainly determined by the superposition of scattered light by nanoparticles. If the substrate thickness is increased to 20 nm, the radiation field excited by the substrate can couple with the LSPR fields excited by nanoparticles. When the substrate thickness is up to 140 nm, both the evanescent field of TE_0 waveguide mode and the radiation field excited by the substrate can couple with the LSPR fields excited by nanoparticles. In Fig. 2(b), two obvious peaks occur when the substrate thicknesses are 20 nm and 140 nm, respectively. However, there is only one peak when the substrate thickness is 0 nm. From Fig. 2(b), it is obvious that the full width at half maximum (FWHM) becomes remarkably narrow within the wavelength range from 650 nm to 900 nm and the corresponding peak value shows remarkable enhancement within the wavelength range from 500 nm to 650 nm as the substrate thickness increases. These phenomena can be explained by the field coupling theory. The interference among the evanescent field, the radiation field, and the LSPR fields is stronger than that between the radiation field and the LSPR fields.

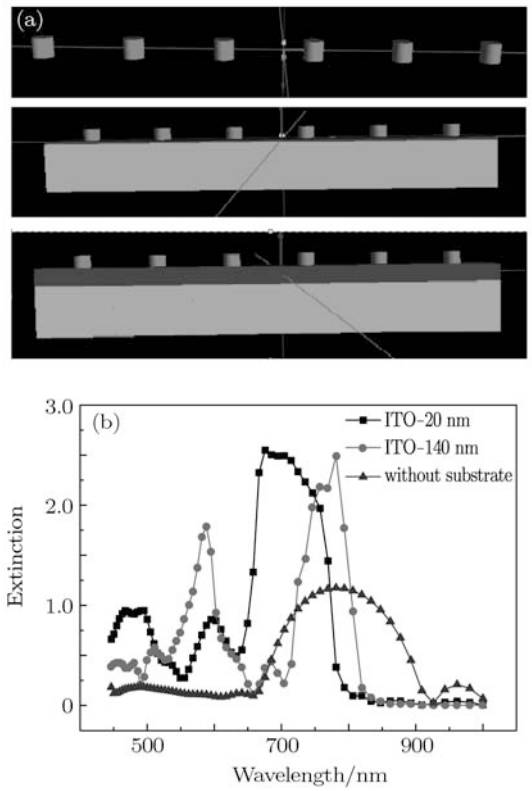


Fig. 2. Schematic diagram of FDTD simulation: (a) periodic gold nanoparticles arrays on the ITO with different thicknesses and (b) extinction spectra of the nanostructure with different thicknesses of substrates.

Secondly, we further investigate the influence of different dielectric constants of the substrate on extinction spectra. The dielectric constants of the sub-

strate are assumed as 1.5, 2.5, 3.6, 10, and 20, respectively, and its thicknesses are 20 nm and 140 nm, respectively. According to formula (1), the 20-nm thick substrate cannot support any waveguide mode when the dielectric constants are 1.5, 2.5, and 3.6, respectively. However, TE_0 waveguide mode can be supported when the dielectric constants are 10 and 20. The 140-nm thick substrate can support TE_0 waveguide mode when the dielectric constant is 3.6 and support both TE_0 and TE_1 waveguide modes when the dielectric constant is 10. All the simulation results are shown in Fig. 3. We arrange the curves in the graphs according to the number of waveguide modes that exist in the substrate. Figures 3(a), 3(b), and 3(c) show the extinction spectra of the substrates that support non-waveguide mode, one waveguide mode, and two waveguide modes, respectively. It is found that the number of peaks increases as the number of waveguide modes increases. The phenomenon could be explained by the field couple theory. When more fields originating from the waveguide couple with LSPR fields, more interference will appear. To further confirm our conclusion, we design a model for the substrate that can support more waveguide modes. As a result, more peaks appear in extinction spectra, as shown in Fig. 3(d). Here, the thickness and dielectric constant of the substrate are 140 nm and 15, respectively. It can be seen from Fig. 3(c) that the FWHM of the spectrum is narrowed to only 10 nm in the wavelength range from 500 nm to 800 nm. This novel feature may attract considerable attention in the future in optical information science and technology, such as optical switching.

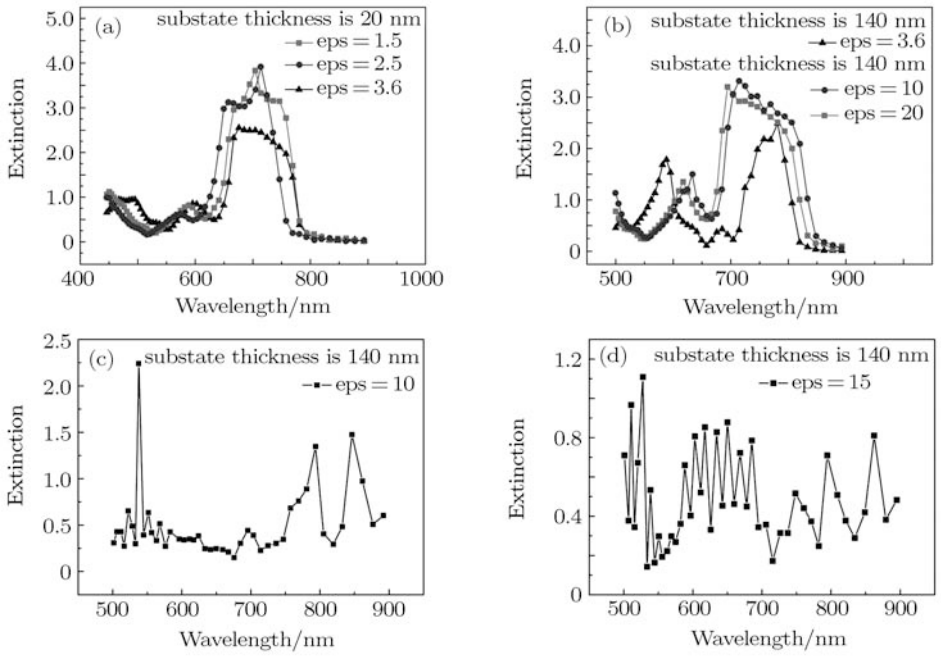


Fig. 3. Extinction spectra of periodic gold nanoparticles arrays on the substrate supporting different numbers of waveguide modes: (a) non-waveguide mode, (b) one-waveguide mode, (c) two-waveguide modes, and (d) multi-waveguide modes.

3. Effect of topologic shape and polarization direction of incident light

In order to investigate the influence of topologic shapes of gold nanoparticles and polarization directions of incident light on extinction spectra, we choose ten topologic shapes. The ten topologic shapes are divided into four groups according to the similarity of the shapes of nanoparticles. Both TE and TM polarization of incident light are used in this work. The structure in our simulations is the same as that in Fig. 1. Here, the size of nanoparticles is in the range of 50 nm to 100 nm. The thickness and dielectric constant of the ITO substrate are 140 nm and 3.6, respectively. The wavelength of the incident light ranges from 500 nm to 750 nm.

Figure 4(a) shows two arrangements of the periodic diamond-like nanoparticle arrays. One of the

long symmetry axis of the nanoparticle is vertical to the X axis, while the other is parallel to X axis. The extinction spectra of the two arrangements are shown in Fig. 4(b) (TM polarization) and Fig. 4(c) (TE polarization), respectively. Though the ratio of short and long axes of the diamond-like shape is 2:3, there is no obvious difference in the extinction spectra for each polarization direction.

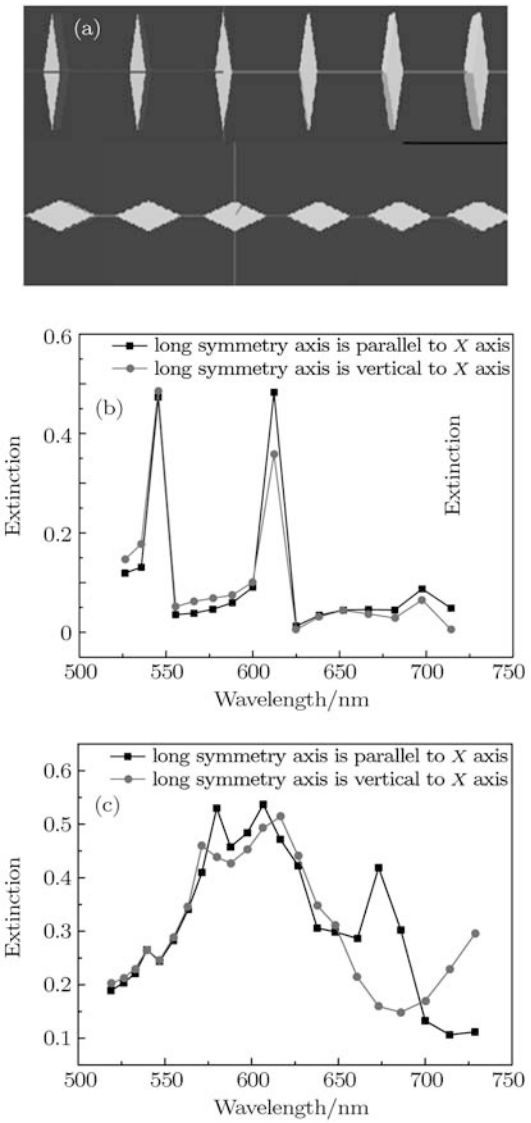


Fig. 4. (a) Schematic diagram of periodic diamond-like nanoparticles arrays. In the upper figure, the long symmetry axis of the diamonds is vertical to the X axis, while in the lower one it is parallel to the X axis. (b) Extinction spectra of both cases are obtained by TM polarization. (c) Extinction spectra of both cases are obtained by TE polarization.

Group B includes three ring shapes: rectangular, pentagonal, and circular rings, as shown in Fig. 5(a). The radii of the inscribed circles of these ring shapes are all the same, as are the radii of the circumscribed circles. Their extinction spectra are shown in Fig. 5(b) (TM polarization) and Fig. 5(c) (TE polarization).

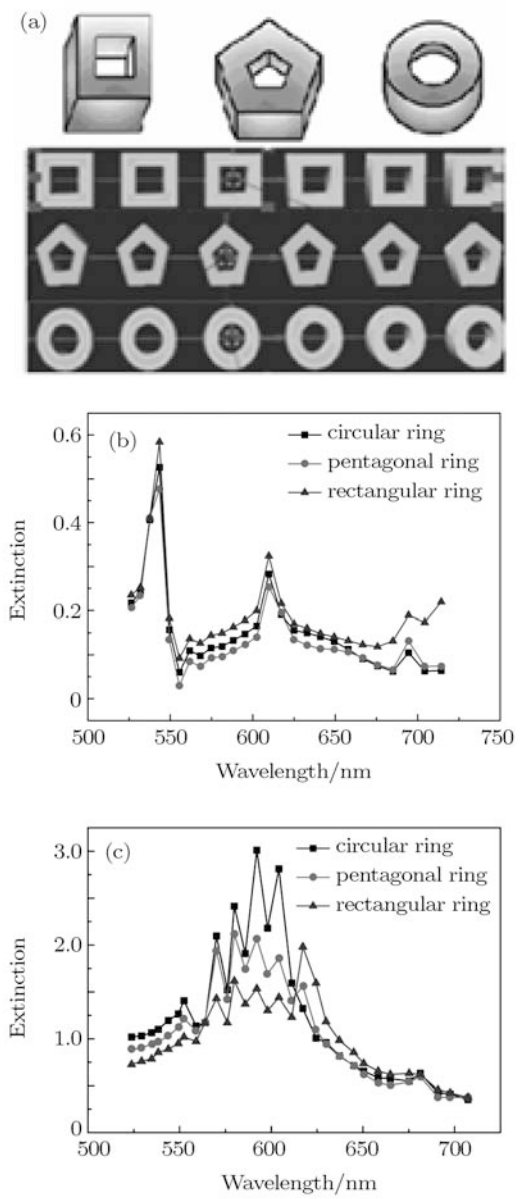


Fig. 5. (a) Schematic diagram of periodic ring shape nanoparticles arrays (rectangular ring, pentagonal ring, circular ring), (b) extinction spectra of them are obtained by TM polarization, and (c) extinction spectra of them are obtained by TE polarization.

Figure 6(a) shows the morphology of Group C, including five-pointed star and flower-like shapes with the same radii of circumscribed circles. The structure of the flower-like shape with four leaves is smoother than that of the five-pointed star shape with five vertices of a pentagon, resulting in their extinction spectra appearing to be obviously different, as revealed in Fig. 6(b) (TM polarization) and Fig. 6(c) (TE polarization).

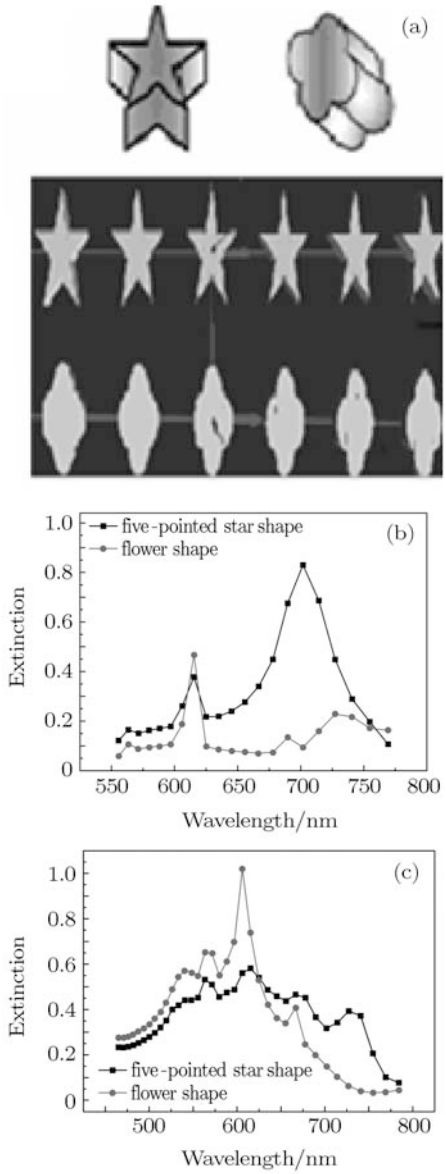


Fig. 6. (a) Schematic diagram of five-pointed star and flower shape periodic nanoparticle arrays, (b) extinction spectra of five-pointed star and flower-like shapes obtained by TM polarization, and (c) extinction spectra of five-pointed star and flower-like shapes obtained by TE polarization.

Group D includes letters L, Y, T, and X, which are non-closed shapes, as shown in Fig. 7(a). The corresponding extinction spectra are shown in Fig. 7(b) (TM polarization) and Fig. 7(c) (TE polarization).

From the discussion above, we can draw the following conclusions. First, there is a slight change in extinction spectra of the nanostructures when the nanoparticles have similar shapes. In particular, in the TM polarization case, extinction spectra are very similar in Groups A, B, and D. Second, the extinction spectra in Group C exhibit different optical properties, indicating that the extinction properties are shape-dependent. Third, the positions of the peaks and the line shapes of the extinction spectra caused by TM polarization are greatly different from those caused by TE polarization. For all nanostructures, extinction the spectra show more oscillation for TE polarization than those for TM polarization. This should be ascribed to more complicated field coupling caused by TE polarization.

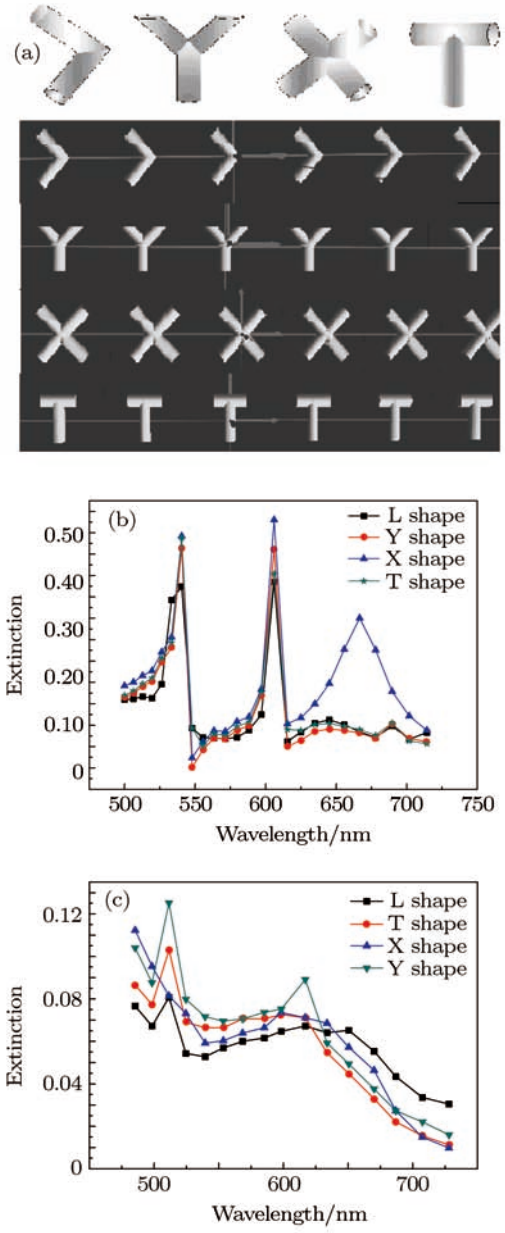


Fig. 7. (a) Schematic diagram of L, Y, X, and T shaped periodic nanoparticles arrays, (b) extinction spectra of them obtained by TM polarization, and (c) extinction spectra of them obtained by TE polarization.

4. Conclusion

In summary, the extinction spectra of the nanostructures composed of periodic gold nanoparticle ar-

rays and the substrate have been investigated by using the FDTD method. The results show that both the thickness and the dielectric constant of the substrate have a great influence on extinction spectra. The number of peaks of extinction spectra becomes large and the line shape of the extinction spectra becomes complicated with an increase in the number of waveguide modes supported by the substrate. We can use field coupling theory to explain these phenomena. Extinction spectra of the structures with ten topologic shapes of gold nanoparticles are also discussed. The results indicate that there is a slight change in the extinction spectra when the nanoparticles have similar shapes. It is found that for all nanostructures, he extinction spectra show more oscillation for TE polarization than those for TM polarization. This should be ascribed to more complicated field coupling caused by TE polarization.

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