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Multiple Fano resonances in nanorod and nanoring hybrid nanostructures*

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Multiple Fano resonances of plasmonic nanostructures have attracted much attention due to their potential applications in multicomponent biosensing. In this paper, we propose a series of hybridized nanostructures consisting of a single nanoring and multiple nanorods to generate multiple Fano resonances. One to three Fano resonances are achieved through tuning the number of nanorods. The interaction coupling process between different components of the nanostructures is recognized as the mechanism of multiple Fano resonances. We also theoretically investigate the applications of the produced multiple Fano resonances in refractive index sensing. The specific properties of multiple Fano resonances will make our proposed nanostructures beneficial to high-sensitivity biosensors.

Keywords: multiple Fano resonances, plasmonic coupling, biosensors, hybrid nanostructures

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1. Introduction

Plasmonic resonances, the collective oscillation of free electrons, of metallic nanostructures have the ability to concentrate the incident light beyond the optical diffraction limitation and significantly enhance the intensity of the localized electromagnetic field, which enables plasmonic nanostructures to be applied in color printing, luminescence enhancement, optical security, and photovoltaic devices.[1–5] Therefore, optical properties of plasmonic nanostructures have attracted much attention. Specifically, nonlinear optical properties of plasmonic nanostructures, such as Fano resonance, electromagnetic induced transparency, and Rabi splitting, have been intensively investigated.[6–10] Among these nonlinear phenomena, Fano resonances have aroused great interest for their specific characteristics of narrow full width at half maximum, high quality factor, and sensitive response to the change of refractive index of the surrounding medium, and therefore find wide applications in nanoelectronics, displays, and biosensors.[11–14]

Fano resonance was firstly recognized as a specific phenomenon in the quantum domain.[15] However, more and more reports about Fano resonances and their applications have been demonstrated in the nanophotonic area with the development of nanofabrication technologies, including focused ion beam and electron beam lithography.[16–18] In nanophotonics, Fano resonances are produced by plasmonic couplings between neighboring nanoparticles. The coupling process will produce a superradiant bonding mode (nanoparticles oscillating in phase) and a subradiant antibonding mode (out of phase). The broad superradiant mode overlaps with the sharp subradiant mode and forms a Fano resonance.[19,20] Since Fano resonances have been introduced into the plasmonic area, different shapes of metallic nanostructures have been intensively proposed to generate Fano resonances, such as 'XI'-shaped nanoclusters,[21] asymmetric nanodisks,[22] nanodisk oligomers,[23] nanoring oligomers,[24] and split ring resonators.[25] Recently, dielectric nanostructures made of silicon or TiO_2 were also demonstrated to produce Fano resonances.[26,27]

In comparison to plasmonic nanostructures with single Fano resonance, nanostructures producing multiple Fano resonances are of interest due to their different responsibility to multiple components of the surrounding environments and potential applications in multicomponent biosensing.[28] Therefore, how to produce multiple Fano resonances is beneficial to biosensors for multicomponent analysis. Here, we propose a series of hybrid nanostructures consisting of a single nanoring and multiple nanorods to produce multiple Fano resonances. One to three Fano resonances are sequentially demonstrated with tuning the number of nanorods. A plasmonic hybridization model is employed to analyze the coupling mechanism of these Fano resonances. We also theoretically investigate the applications of our proposed multiple Fano resonances in refractive index sensors.

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2. Theoretic model

The proposed hybrid nanostructures that produce one/multiple Fano resonances are composed of a single nanoring and one/multiple nanorods. The schematic illustration of the hybrid nanostructure for one Fano resonance is shown in Fig. 1(a). A nanorod and a nanoring sit side by side with a gap (g). The polarization direction is vertical, and these nanostructures resonate as dipole modes. They couple and hybridize to form hybridization modes. By adding extra nanorods to the right side of the hybrid nanostructure in Fig. 1(a), more complex coupling processes will be induced to produce multiple Fano resonances.

We will discuss the mechanism of the multiple Fano resonances with simulation of the near-field electric field and charge density distributions with commercial finite-difference time-domain software. A plane wave with vertical polarization is utilized as incident light, and the wavelength range is selected as 500 nm to 3000 nm. Perfect matching layers are adopted as the boundary conditions, and the step sizes of calculations are $5 \times 5 \times 5$ nm^3. The substrate is quartz with a refractive index of 1.4, and the dielectric function for gold is extracted from Johnson and Christie's data.[29]

3. Results and discussion

3.1. Single Fano resonance

Figure 1(a) shows the schematic illustration of our proposed nanostructure for producing single Fano resonance, which consists of one nanorod and one nanoring. For easy description, we term the hybrid nanostructure in Fig. 1(a) as NRD. The height (h) of the nanoring and nanorod is fixed as 50 nm, and the inner (r_{in}) and outer (r_{out}) radii of the ring are 150 nm and 200 nm, respectively. The gap (g) is 50 nm, and the length (l) and width (w) of the nanorod are 500 nm and 40 nm, respectively. Figure 1(b) presents the calculated extinction and absorption spectra of the NRD. In this work, extinction is defined as '1-transmission', while absorption refers to 'extinction–reflectance'. It can be seen that the extinction dip is located at the position of the absorption peak, which clearly illustrates that the extinction dip (C) is a Fano resonance dip.

In order to investigate the mechanism of the Fano resonance in the NRD, we separately simulate the extinction spectra of the nanorod and nanoring, as shown in Figs. 2(a) and 2(c). The corresponding charge density distributions (see the insets of Figs. 2(a) and 2(c)) demonstrate that both nanorod and nanoring resonate as dipole modes, in which the red color represents positive charge, while the blue color is negative charge. When we put them closely together, these two dipole modes will hybridize and form two peaks, marked as A and B. For peak A, the nanorod and nanoring oscillate in phase, while they are out of phase for peak B, as shown in Fig. 2(b). It is well known that coupled nanoparticles oscillating in phase form a bright mode (superradiant bonding mode), while they are out of phase in dark mode (subradiant antibonding mode).[30–32] Therefore, peak A is a bright mode, and peak B is a dark mode. Hence, the superradiant mode (A) overlaps with the subradiant mode (B) and forms a Fano resonance.

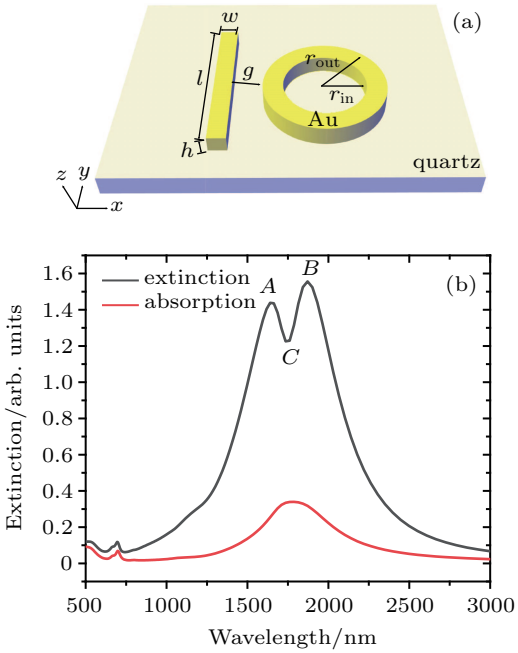


Fig. 1. (a) Schematic of the NRD nanostructure consisting of one nanoring and one nanorod. (b) The extinction and absorption spectra of the NRD.

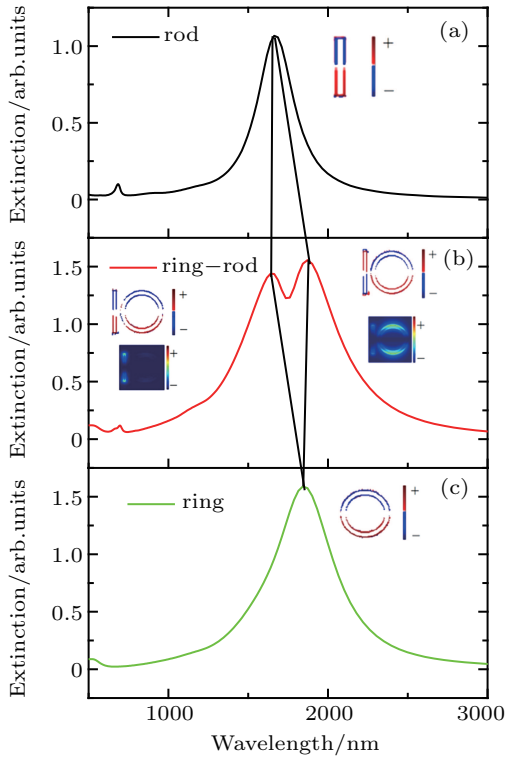


Fig. 2. The mechanism of Fano resonance in the NRD nanostructure. Extinction spectra of the (a) nanorod, (b) NRD, and (c) nanoring. Insets are the near-field charge density and electric field distributions.

3.2. Two Fano resonances

In the following parts, we increase the number of nanorods and make the nanoring sequentially couple with these nanorods to form multiple Fano resonances. First, we add an extra nanorod to the right side of the NRD nanostructure and the triple-nanoparticle cluster is termed as NRDD, as shown in Fig. 3(a). The width of the right nanorod is $w_2 = 40$ nm, and the length is $l_2 = 350$ nm, which is shorter than that of the left nanorod ($l_1 = 500$ nm). The gap (g_2) between the ring and right nanorod is 50 nm, and the remaining parameters are the same as those of the NRD in Fig. 1. Figure 3(b) gives the simulated extinction and absorption spectra of the NRDD. Three distinct peaks (marked as *A*, *B*, and *C*) are observed, and two absorption peaks (labeled as *D* and *E*) are located on the rising or falling edges of the extinction peaks, which are direct evidence of Fano resonances.[31] Therefore, two Fano resonances are achieved with two different lengths of nanorods coupling to the central nanoring.

To investigate the underlying physics of these two Fano resonances, we calculate the near-field electric field and charge density distributions of the corresponding peaks in Fig. 3(b). As shown in Fig. 4(a), the left nanorod and the central nanoring oscillate in phase, and they are recognized as a unit (NRD). Therefore, the NRD couples with the right nanorod and forms peaks *A* and *B*. For peak *A*, the NRD is in phase with the right nanorod, while they are out of phase for peak *B*. Therefore, peaks *A* and *B* represent the bright and dark modes, respectively. These two modes overlap and form a Fano resonance.[33–35] Interestingly, the charge density distribution of the central nanoring is out of phase with that of the left and right nanorods for peak *C* (Fig. 3(b)), demonstrating its nature of dark mode. Its corresponding bright mode should have the central nanoring oscillating in phase with that of the right and left nanorods, which is the same as the charge density distribution of peak *A*. Therefore, dark mode *C* overlapping with the bright mode *A* forms the second Fano resonance. The hybridizing processes are changed and two Fano resonances are observed when we add an extra nanorod close to the NRD.

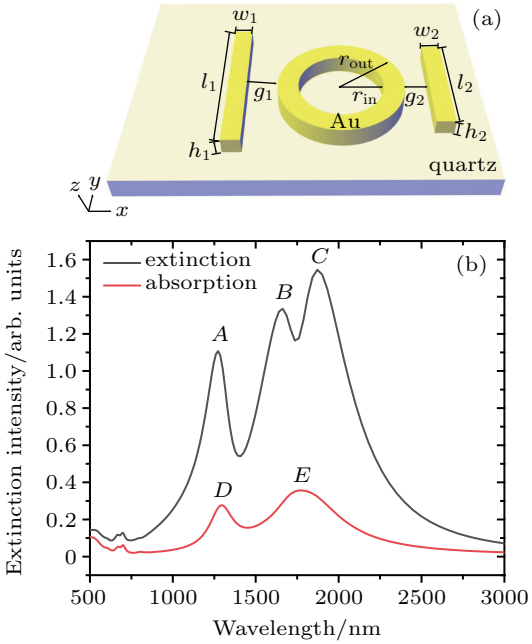


Fig. 3. (a) A unit cell of the NRDD nanostructure consisting of one nanoring and two nanorods. (b) The extinction and absorption spectra of the NRDD.

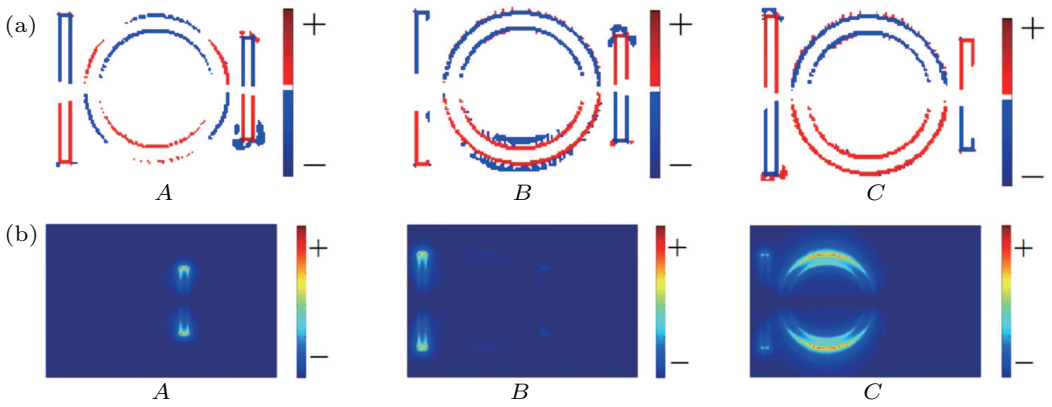


Fig. 4. (a) The charge density and (b) electric field distributions of peaks *A*–*C* of the NRDD in Fig. 3.

3.3. Three Fano resonances

When we continually add an additional nanorod to the NRDD, a more complex plasmonic coupling process will be observed and more Fano resonances can be achieved.[36,37] As shown in Fig. 5(a), a third nanorod is added to the right side of the NRDD, and the new nanostructure is termed as NRDDD. The parameters of the NRDDD are set as follows: $l_3 = 600$ nm, $w_3 = 40$ nm, $g_3 = 50$ nm, and all other parameters are the same as those of the NRDD. Four peaks (marked as *A*, *B*, *C*, and *D*) are observed in the extinction spectrum of NRDDD, as shown in Fig. 5(b). Three absorption peaks (labeled as *E*, *F*, and *G*) are located at the rising or falling edges

of the extinction peaks. Therefore, three Fano resonances are obtained in NRDDD.

Figure 6 gives the electric field and charge density distributions of peaks *A*–*D* in the NRDDD. Peak *A* is a bright mode because all of these four nanoparticles are oscillating in phase. For peak *B*, the smallest nanorod is out of phase with the other three nanoparticles, indicating that peak *B* is a dark mode. For peak *C*, the main coupling is among the NRDD, in which the central nanoring couples with the two nanorods and forms a dark mode. Overall, the newly added nanorod does not apparently influence the electric field distributions of peaks *A*–*C*, and the main coupling processes are similar to that of the NRDD. Therefore, these two dips between peak *A* and *C* are Fano resonance dips. Meanwhile for peak *D*, the main coupling process is between the newly added nanorod and the NRDD. Peak *D* is a dark mode, because the newly added nanorod is out of phase with the NRDD. The corresponding bright mode (the NRDD oscillating in phase with the newly added nanorod) is peak *A*. Therefore, the third Fano resonance is formed due to the overlap between peaks *A* and *D*.

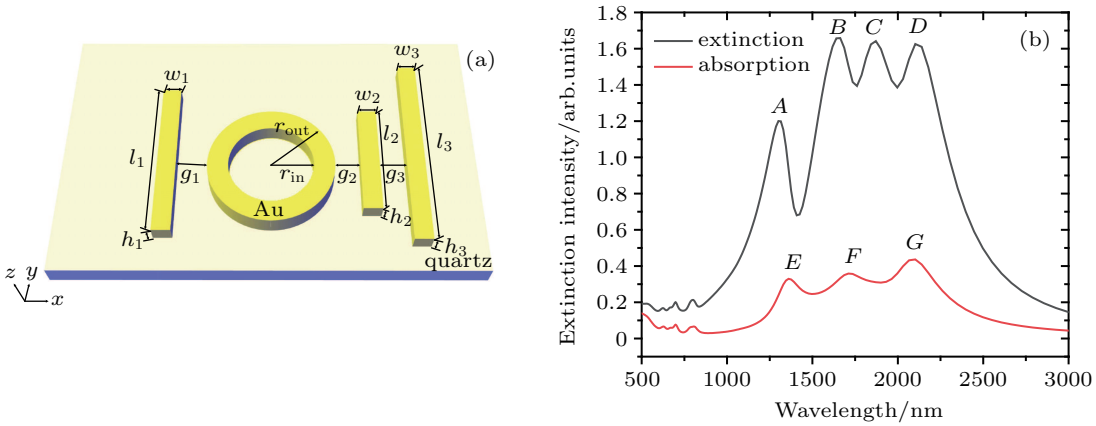


Fig. 5. (a) Schematic illustration of the NRDDD consisting of one nanoring and three nanorods. (b) The extinction and absorption spectra of the NRDDD.

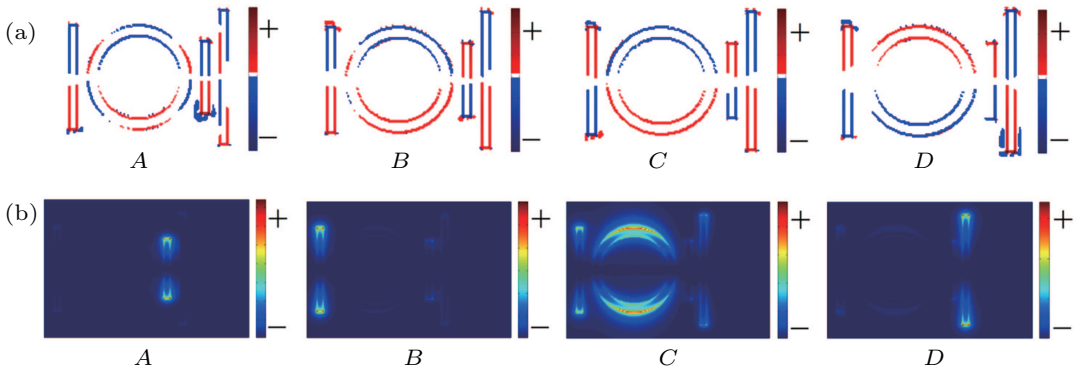


Fig. 6. (a) The charge density and (b) electric field distributions of peaks *A*–*D* of the NRDDD in Fig. 5.

3.4. Theoretical analysis of applying multiple Fano resonances in biosensing

We also theoretically investigate the applications of the proposed two Fano resonance nanostructure (NRDD) in biosensing. Figure 7(a) gives the simulation results. As the refractive index of the ambient medium around the NRDD increases, the two Fano resonance dips (labeled as *a* and *b*) are gradually red-shifted. We calculate the sensitivity for these two Fano resonance dips, as shown in Fig. 7(b). The sensitivities and the figures of merit for these two Fano resonance dips are 1195 nm/RIU and 1380 nm/RIU, 8.5 and 18.9, respectively. Compared with the Fano resonance at short wavelength in Fig. 7(a), the longer wavelength Fano resonance is more sensitive to the ambient refractive index. In addition to the refractive index shifts for biosensing, another potential sensing application is the detection of different molecules through the plasmon–exciton coupling between the plasmonic Fano resonances and excitons of molecules. In the plasmon–exciton coupling process, an absorption or Rabi split dip will appear in the Fano resonance dips when we tune the Fano resonance in the position of the absorption or exciton mode of molecules. In this case, multiple Fano resonances can be applied to detect appropriate multiple components of the environment. Therefore, the proposed plasmonic nanostructures

with multiple Fano resonances may be applied in refractive index biosensing and multicomponent analyzing.

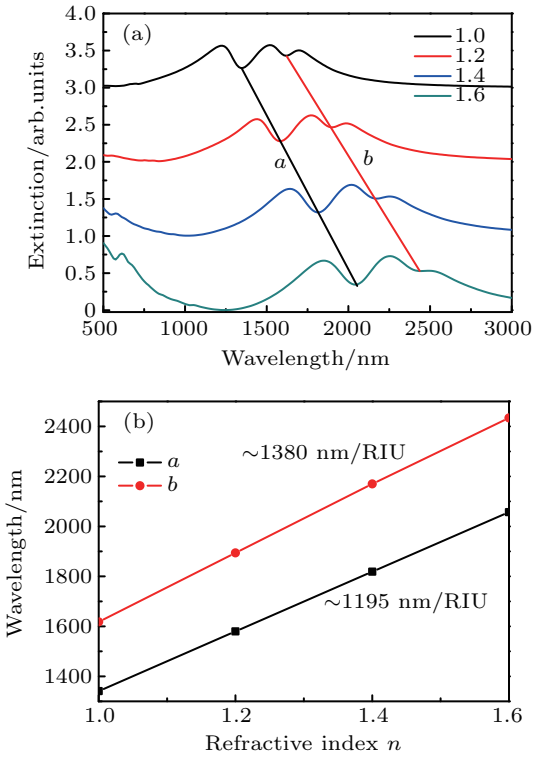


Fig. 7. (a) Refractive index sensing with multiple Fano resonances of the NRDD. (b) The calculated sensitivity of Fano resonances in the NRDD.

4. Conclusion and perspectives

In this paper, multiple Fano resonances of nanostructures consisting of one single nanoring and different numbers of nanorods and their underlying physics are theoretically investigated. With the help of a plasmonic hybridization model, we decompose the multiple Fano resonances of the proposed nanostructures into different coupling processes between different nanoparticle components. We also apply the proposed multiple Fano resonance in the refractive index-related biosensing. The presented nanostructures and their specific optical properties will be beneficial in plasmonic biosensing and multicomponent analyzing.

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