

Magnetic Fano resonance of heterodimer nanostructure by azimuthally polarized excitation

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Abstract: The optical properties of a Si-Au heterodimer nanostructure, which is composed of an Au split nanoring surrounded by a Si nanoring with a larger diameter, are investigated both theoretically and numerically. It is found that a pure magnetic plasmon Fano resonance can be achieved in the Si-Au heterodimer nanostructure when it is excited by an azimuthally polarized beam. It is revealed that the pure magnetic Fano resonance is generated by the destructive interference between the magnetic dipole resonance of the Si nanoring and the magnetic dipole resonance of the Au split nanoring. A coupled oscillator model is employed to analyze the Fano resonance of the Si-Au heterodimer nanostructure. The pure magnetic response of the Si-Au heterodimer nanostructure is verified by the current density distributions and the scattering powers of the electric and magnetic multipoles. The Fano resonance in the Si-Au heterodimer nanostructure exhibits potential applications of low-loss magnetic plasmon resonance in the construction of artificial magnetic metamaterials.

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1. Introduction

Fano resonance based on artificial plasmon structure has become the focus of research in recent years for its wide applications in the areas such as surface enhanced Raman scattering (SERS) [1], slow-light devices [2], biological and chemical sensors [3,4], optical switch [5,6], and plasmon ruler [7]. Fano resonance, exhibiting an asymmetric line shape and inducing a large electromagnetic field enhancement [8,9], results from the interactions of narrow subradiant modes and broad superradiant modes. So far, numerous nanostructures have been designed to generate Fano resonance, such as nanoparticle clusters [10–13], dolmen structures [14–16], nonconcentric ring/disk cavities [17,18], core-shell structures [19–22].

Due to the deficiency of natural magnetism in metal nanomaterials at optical frequencies, the initial Fano resonance was studied mainly based on the pure electric responses in metal nanostructures. And then researchers began to focus on magnetic-based Fano resonance due to its potential application of artificial magnetism. The magnetic-based Fano resonance had been studied in many plasmonic structures. Wang et al. demonstrated that the double Fano resonance effect can be achieved in the SRRs/Rod structure due to the interplay of electric and magnetic plasmon modes [23]. Li et al. observed multiple magnetic Fano resonance in split ring-perfect ring nanostructure [24]. Ci et al. theoretically demonstrated a magneticbased Fano resonance of hybrid silicon-gold nanocavities in the near-infrared region [25]. The magnetic-based Fano resonance generally originates from the coupling between the electric dipole resonance mode and the magnetic dipole resonance mode. However, the dominant scattering from the electric dipole leads to a high radiative loss, which limits its application area. Therefore, the research on the pure magnetic plasmon Fano resonance have become a popular topic. Bao et al. demonstrated that a pure magnetic plasmon Fano resonance can be realized at optical frequency with Au split ring hexamer nanostructure [26]. Miroshnichenko et al. theoretically and experimentally demonstrated that the magnetic Fano resonances can be achieved in the nanoparticle oligomer structures due to the interplay of magnetic responses [27–33].

In this paper, we investigated the optical properties of a Si-Au heterodimer nanostructure (Si-Au HDNS), which is composed of an Au split nanoring (Au SNR) surrounded by a Si nanoring (Si NR) with a larger diameter. An azimuthally polarized beam (APB) is utilized as the incident light source. At each point, the electric field of the APB is linearly polarized but its vector is oriented perpendicularly to the radius vector from the beam axis. In most studies, a plane wave or a focused Gaussian beam was generally used as the incident light source, which was either linearly or circularly polarized. Recently, it was shown that the APB has the capability to effectively excite the magnetic dipole resonance and suppress the electric dipole resonance of the nanostructure [34]. In this way, the magnetic dipole resonances of the Si NR and Au SNR can be excited effectively, resulting in the generation of the pure magnetic plasmon Fano resonance. We have demonstrated that a pure magnetic Fano resonance can be achieved in a Si-Au HDNS excited by an APB. It is shown that the pure magnetic Fano resonance of the Si NR

and the magnetic dipole resonance of the Au SNR. These two interacting modes could be regarded as two coupled oscillators, a coupled oscillator model is employed to analyze the Fano resonance of the Si-Au heterodimer nanostructure. The wavelength as well as intensity of the Fano resonance can be adjusted effectively by tuning the geometry parameters of the Si-Au HDNS. Due to the interplay of the two magnetic modes, magnetic hybridization with reduced radiative loss can be realized, which could be beneficial to the development of low loss plasmonic applications such as low-loss sensors.

2. Structures and simulation method

The three-dimensional and two-dimensional schematic diagrams of the Si-Au HDNS are shown in Figs. 1(a) and 1(b), respectively. The inner and outer radius of the Au SNR is r_1 and r_2 , located at the center of the Si NR with the inner radius r_3 , outer radius r_4 . The thickness of the Si NR and the Au SNR are both T, and the gap length of Au SNR is g. The dielectric constants of gold and silicon are taken from Refs [35] and [36], respectively.

The numerical simulations are performed by the finite difference time domain (FDTD) Solutions software. The APB source is utilized as the incident light propagating in z direction, at each point, the electric field of the APB is linearly polarized but its vector is oriented perpendicularly to the radius vector from the beam axis. Figure 1(c) shows the intensity and electric vector distributions of the APB. To avoid the interference of the reflection from the boundaries, we set perfect match layers (PML) outside the nanostructure to absorb all electromagnetic waves inside the PML. The refractive index of the surrounding is 1.



Fig. 1. (a) Three-dimensional and (b) two-dimensional schematic diagrams for the Si-Au HDNS with the descriptions of the geometrical parameters. (c) Intensity and electric vector distributions of the APB.

3. Results and discussion



Fig. 2. (a) Scattering spectra of the Si NR with the illumination of the APB. (b) The field enhancement and current density distributions of the Si NR at 868nm.

First of all, the optical properties of the Si NR and the Au SNR are investigated. In consideration of plasmon coupling intensity, the parameters of the Si-Au HDNS are set as: $r_1 = 45$ nm, $r_2 = 85$ nm, $r_3 = 110$ nm, $r_4 = 160$ nm, g = 35 nm and T = 100 nm. An APB source is utilized as the incident light propagating in z direction. It is shown that the magnetic dipole could be excited effectively in both of the Si NR and Au SNR. As shown in Fig. 2, for the Si NR, only the magnetic dipole mode centered at 868 nm can be excited by the APB. The magnetic dipole mode is characterized by circular displacement currents on the Si NR, which is similar to that described for a silicon hollow nanodisk [37]. For the Au SNR, as shown in Fig. 3, there is a sole resonance peak at 874 nm, corresponding to the magnetic dipole mode, which is characterized by induced antisymmetric circular displacement currents on the two half rings. This induced magnetic mode couples weakly to the external optical field and could not be excited directly under a linearly polarized beam at normal incidence [38], but it could be efficiently excited by the APB.



Fig. 3. (a) Scattering spectra of the Au SNR with the illumination of the APB. (b) The field enhancement and current density distributions of the Au SNR at 874 nm.

We also calculated the scattering spectra of the Si-Au HDNS excited by the APB in order to better understand its optical properties. When the Si NR and Au SNR are aligned together to form a heterodimer nanostructure, one can see that a representative Fano resonance spectral response with its dip at 842 nm and peaks at 759 and 996 nm respectively appears in Fig. 4(a). The Fano resonance results from the interaction between a narrow magnetic mode and a broad magnetic mode. The field enhancement and current density distributions of the resonance dip are presented in Fig. 4(c), and the field enhancement and current density

distributions of the resonance peaks are presented in Figs. 4(b) and 4(d), respectively. From the viewpoint of plasmon hybridization theory, the coupling between the two plasmon modes results in splitting of the modal energies into bonding and anti-bonding resonances [39]. One can see that the resonance with a higher energy around 759 nm is the anti-bonding dipoledipole mode, and the resonance with a lower energy around 996 nm is the bonding dipoledipole mode. It can be found that the field enhancement is mainly concentrated in the gap of the Au SNR and the space between the Si NR and Au SNR, which represents the strong coupling between the Si NR and Au SNR. It is demonstrated that Fano resonance derives from the interaction of magnetic dipole modes, judging from their current density distributions.



Fig. 4. (a) Scattering spectra (left panel) of the Si NR (bottom), Au SNR (middle) and Si-Au HDNS (top) with the illumination of the APB. (b) and (d) show the field enhancement and current density distributions (right panel) of the resonance peaks. (c) shows the field enhancement and current density distributions (right panel) of the resonance dip.

The Fano resonance of the Si-Au HDNS excited by the APB can be interpreted as the interference between a broad magnetic mode and a narrow magnetic mode. These two interacting modes could be regarded as two coupled oscillators, the two oscillators provide

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the bonding mode and anti-bonding mode. The equation governing the motions of the two oscillators can be written as [40-42]:

$$\frac{d^{2}x_{a}}{dt^{2}} + \gamma_{a}\frac{dx_{a}}{dt} + \omega_{a}^{2}x_{a} + gx_{b} = \frac{1}{2}\left(\eta_{b}\frac{d^{3}x_{b}}{dt^{3}} + \eta_{a}\frac{d^{3}x_{a}}{dt^{3}}\right) + \eta_{a}E$$

$$\frac{d^{2}x_{b}}{dt^{2}} + \gamma_{b}\frac{dx_{b}}{dt} + \omega_{b}^{2}x_{b} + gx_{a} = \frac{1}{2}\left(\eta_{b}\frac{d^{3}x_{b}}{dt^{3}} + \eta_{a}\frac{d^{3}x_{a}}{dt^{3}}\right) + \eta_{b}E$$
(1)

where $\omega_{a(b)}$, $\gamma_{a(b)}$ and $\eta_{a(b)}$ are the resonance frequency, nonradiative damping and radiation coupling efficiency of the anti-bonding (bonding) mode, respectively. g represents the coupling constant between the two oscillators and E denotes as $E = E_0 e^{i\omega t}$ is the electrical field of the excitation beam. The motions of two oscillators are harmonics with forms of $x_{a(b)} = C_{a(b)} e^{i\omega t}$, where $C_{a(b)}(\omega)$ can be analytically derived

$$C_{a}(\omega) = \frac{\left(g + \frac{i}{2}\eta_{b}\omega^{3}\right)C_{b}(\omega) - \eta_{a}E_{0}}{\omega^{2} - i\gamma_{a}\omega - \omega_{a}^{2} - \frac{i}{2}\eta_{a}\omega^{3}}$$
$$-\eta_{a}E_{0}\left(g + \frac{i}{2}\eta_{a}\omega^{3}\right) - \eta_{b}E_{0}\left(\omega^{2} - i\gamma_{a}\omega - \omega_{a}^{2} - \frac{i}{2}\eta_{a}\omega^{3}\right)$$
$$\left(\omega^{2} - i\gamma_{a}\omega - \omega_{b}^{2} - \frac{i}{2}\eta_{b}\omega^{3}\right)\left(\omega^{2} - i\gamma_{a}\omega - \omega_{a}^{2} - \frac{i}{2}\eta_{a}\omega^{3}\right) - \left(g + \frac{i}{2}\eta_{b}\omega^{3}\right)\left(g + \frac{i}{2}\eta_{a}\omega^{3}\right)$$
(2)

These values can be utilized to calculate $\sigma_{sca} = I_0 + |C_a + C_b|^2$ with I₀ accounting for the background, which is used to describe the scattering spectrum of the Si-Au HDNS. As shown in Fig. 5, a good agreement between the theory (red solid curves) and simulation (blue dots) is achieved.



Fig. 5. Scattering spectra of the Si-Au HDNS excited by the APB, where the blue dots and red solid curves are the simulation and fitting results, respectively.

In order to further testify the optical scattering is dominated by the magnetic response, simulated densities of induced electrical currents were used to calculate scattered powers of the electric and magnetic multipoles, which are represented as [43]:

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$$I = \frac{2\omega^4}{3c^3} |\mathbf{p}|^2 + \frac{2\omega^4}{3c^3} |\mathbf{m}|^2 + \frac{\omega^6}{5c^5} \sum |\mathbf{Q}_{\alpha\beta}|^2 + \frac{\omega^6}{20c^5} \sum |\mathbf{M}_{\alpha\beta}|^2$$
(3)

where c is the speed of light, ω is the frequency of light and α , $\beta = x$, y, z. And the first and second terms originate from the electric and magnetic dipole scattering. The third and fourth terms correspond to the electric and magnetic quadrupole scattering. In the multipole expansion, the polarization current $J_P = \partial P/\partial t$ was used as the induced volume current j, which had the form $-i\omega P = -i\omega\epsilon_0(\epsilon_r-1)E$ in the case of harmonic excitation $-\exp(-i\omega t)$. Based on the current distribution, the electric dipole (p), magnetic dipole (m), electric quadrupole ($Q_{\alpha\beta}$), and magnetic quadrupole ($M_{\alpha\beta}$) can be expressed on a Cartesian basis (α , $\beta = x$, y, z) as follows [44,45]:

$$\mathbf{p} = \frac{1}{-i\omega} \int \mathbf{j} d^3 \mathbf{r} \tag{4}$$

$$\mathbf{m} = \frac{1}{2c} = \int (\mathbf{r} \times \mathbf{j}) d^3 \mathbf{r}$$
 (5)

$$Q_{\alpha\beta} = \frac{1}{-2i\omega} = \int \left[r_{\alpha} j_{\beta} + r_{\beta} j_{\alpha} - \frac{2}{3} (r \cdot j) \delta_{\alpha\beta} \right] d^{3}r$$
(6)

$$\mathbf{M}_{\alpha\beta} = \frac{1}{3c} \int \left[\left(\mathbf{r} \times \mathbf{j} \right)_{\alpha} r_{\beta} + \left(\mathbf{r} \times \mathbf{j} \right)_{\beta} r_{\alpha} \right] d^{3}r$$
(7)



Fig. 6. Scattering power of the multipoles as a function of the wavelength, the contributions of the magnetic dipole (MD), electric dipole (ED), magnetic quadrupole (MQ), and electric quadrupole (EQ) to the total scattering are revealed.

Figure 6 shows the scattering powers of the multipoles in the Si-Au HDNS, which reveals the contributions of the magnetic dipole (MD), electric dipole (ED), magnetic quadrupole (MQ), and electric quadrupole (EQ) to the total scattering. It is demonstrated that magnetic dipole scattering dominates the total scattering, validating the pure magnetic response of the Si-Au HDNS.



Fig. 7. Scattering cross sections of the Si-Au HDNS with (a) different Au SNR inner radius r_1 and (b) different Si NR outer radius r_4 .

In order to get insight into the origins of the resonances, we further investigate the effects of the outer radius of the Si NR (r_4), the inner radius of the Au SNR (r_1), the gap length of the Au SNR (g), and the thickness of the rings (T) on the spectra position and intensity of the Fano resonances. In Fig. 7, we investigate the resonance wavelength and intensity of the magnetic Fano resonance by varying the inner radius of the Au SNR (r_1) and the outer radius of the Si NR (r_4). With the increasing of r_1 and r_4 , the scattering spectra of Fano resonance are red shifted obviously.



Fig. 8. The resonance peak wavelengths of the bonding mode and anti-bonding mode versus (a) the gap length of the Au SNR and (b) the thickness of the rings

The relationships between the resonance peak wavelengths of the two coupling modes and the gap length of the Au SNR are shown in Fig. 8(a). One can see that the two coupling modes are blue shifted with the increasing of gap length (g). According to LC circuit resonance model, in U-shaped split ring resonator (SRR), the resonance wavelength is proportional to $(LC)^{1/2}$, where L is the inductance of SRR and C is the capacitance between the two arms which is inversely proportional to the gap length [46]. This explains the phenomenon that resonances exhibit an obvious blueshift with increasing of gap length. In Fig. 8(b), we investigate the resonance peak shift of the bonding mode and anti-bonding mode

with increasing of thickness of the rings. It should be noted that the thickness of the Si NR and Au SNR is changed simultaneously. As shown in Fig. 8(b), the two coupling modes are red shifted when increasing thickness (T) from 80 nm to 150 nm.



Fig. 9. (a) Scattering cross sections of the Si-Au HDNS as a function of the refractive index of the environment. (b) The resonance peak wavelengths of the bonding mode and anti-bonding mode versus the refractive index of the environment.

In order to investigate the sensing performance of the Si-Au HDNS, the scattering spectra with different dielectric environments are shown in Fig. 9(a). Figure 9(b) shows the resonance peak wavelengths of the bonding mode and anti-bonding mode vs. environmental refractive index. The two modes exhibit a red shift with increasing of refractive index. This can be understood by the fact that the resonance wavelength is proportional to the refractive index of the media environment [47]. The sensitivity (resonance peak shift per index refractive of external medium) and figure of merit (FOM = $(\delta\lambda/\delta n)$ /linewidth) were used to describe the spectral shift of resonances and the sensing performance [38]. In order to investigate the sensing performance, the sensitivity and figure of merit are investigated. The sensitivity (450 nm/RIU) and figure of merit (FOM = 6.1) can be obtained at bonding mode, and therefore our low-loss magnetic Fano resonance can be used as a basis for the sensor applications.

4. Conclusion

In summary, we have demonstrated that a pure magnetic Fano resonance can be achieved in a Si-Au HDNS excited by an APB. In this way, the magnetic dipole resonances of the Si NR and Au SNR can be excited effectively, leading to the formation of the pure magnetic plasmon Fano resonance. The wavelength and intensity of the Fano resonance can be adjusted by varying the geometry parameters of the Si–Au HDNS. The tunable magnetic Fano resonance proposed in this work may find potential applications in novel photonic devices such as low-loss sensors.

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