Dual-band unidirectional forward scattering of Au–Si sliced nanorod in the visible region

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Received: 18 March 2019 / Accepted: 2 May 2019 / Published online: 8 May 2019
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Abstract
Strong resonant light scattering by an Au–Si sliced nanorod is investigated by the finite element method (FEM) based on COMSOL Multiphysics. Stemming from the interference between the electric, magnetic and toroidal multimodes in Au–Si sliced nanorod, the forward scattering is enhanced and backward scattering is attenuated substantially in visible region. Moreover, the high-efficiency unidirectional forward scattering is not limited to one specific wavelength but can fit in the multiple wavelengths. The structural parameters have an effect on the enhancement of different multimode resonances.

1 Introduction
Nanoparticles offer diverse functionalities in nano-photonics devices such as field enhancement, surface-enhanced Raman scattering (SERS), imaging and visualization which have attracted interests in the field of light scattering [1–6]. In particular, due to their ability to support resonances known as localized surface plasmons (LSPs) [7, 8], metal nanoparticles concentrate light into nanometric volumes and exhibit significant gain in directivity in the visible regimes. However, the intrinsic ohmic loss in metal nanoparticles leads to low antenna efficiency [9]. Recently, low absorbing dielectrics with large permittivity values have attracted considerable attention as metamaterials to optimize the emission directivity, light switches and photonic devices [10–12]. A dielectric nanoparticle can be regarded as a magnetic dipole scattering subject of the incident electromagnetic wave at the resonant wavelength. The resonance increases the magnetic field around the nanoparticle in the visible region. Although the full dielectric nanoantenna reduces the loss due to materials, its local field enhancement effect is significantly weaker than that of metal nanoantennas.

Research on novel metal–dielectric composite nanoantennas is conducted, designing metal materials to exert their local field enhancement effects, while using dielectric materials to suppress metal loss [13]. With regard to metal–dielectric hybrid nanoparticles, the spectral positions of multimode resonances and local field distributions are determined by the structure, size, and aspect ratio [14–18]. They can be employed to realize strong attenuation of backward scattering and such directional scattering considered as antennas can trap external electromagnetic fields [19–22]. However, most of the previous studies on optical dielectric nanoparticles primarily focus on the structures such as spheres, cubes, or dimer and trimer structures [10, 11, 23, 24]. A spherical geometry has only 2 degrees of freedom, whereas the electromagnetic field enhancement between dimer and trimer depend strongly on the widths of the gaps separating the nanoparticles. Gaps which are too narrow may lead to conductive overlap between two adjacent nanostructures consequently compromising the field enhancements [10]. In comparison, a nanorod structure provides more flexibility in magnetic response tuning and the field enhancement is not affected by the inter-particle coupling spacing [25]. Moreover, in addition to multimode interference, directional scattering can also be achieved by other methods, such as: a single plasmonic trimer and chip-integrated geometric
metasurface, and the scattering direction can be switched by the operating frequency or polarization state [26–28].

Herein, a novel Au–Si sliced nanorod nanoantenna which can support electric dipole (ED), magnetic dipole (MD) and toroidal dipole (TD) is investigated by the finite element method (FEM) based on the COMSOL Multiphysics software. The effects of the radius of the Au–Si sliced nanorod on the different multimode resonances are studied, and forward scattering and backward scattering are evaluated. Moreover, the Au–Si sliced nanorod with vanishing backward scattering can achieve unidirectional forward scattering at multiple wavelength bands, which has large potential in nanoelectronics as nanoantennas and photovoltaic devices [20, 21, 29, 30].

2 Theoretical assessment

A numerical approach of COMSOL Multiphysics based on the finite element method is implemented to calculate the scattering cross-section of a nanoparticle with an arbitrary shaper and constituent multimode contributions. The theoretical investigation starts with multimode decomposition and the regular electric dipole moment $P_{\text{ED}}$ of a scattering event is calculated as [31]:

$$P = \int P(r')dr',$$

and

$$T = \frac{i\omega}{10} \int \left\{ 2r'^2 P(r') - (r' \cdot P(r'))r' \right\} dr',$$

$$Q = 3 \int [r' P(r') + P(r')r']dr',$$

$$M = -\frac{i\omega}{2} \int [r' \times P(r')]dr',$$

$$Q^m = -\frac{2i\omega}{3} \int [r' \times P(r')]r'dr',$$

showing the toroidal dipole moment $T_{\text{TD}}$, electric quadrupole tensor $Q_{\text{EQ}}$, magnetic dipole moment $M_{\text{MD}}$, and tensor of the magnetic quadrupole moment $Q^m_{\text{MQ}}$.

According to Ref. [31], the scattering cross-section $\sigma_{\text{sc}}$ is defined from $P_{\text{sc}}$ by normalization to the energy flux of the incident wave $I_{\text{inc}}$:

$$P_{\text{sc}} \approx \frac{k_0^4}{12\pi\varepsilon_0^2\mu_0} |P + \frac{ik_d}{v_d} T|^2 + \frac{k_0^4 E_d}{12\pi\varepsilon_0 v_d} |M|^2$$

$$+ \frac{k_0^6 E_d}{1440\pi\varepsilon_0 v_d \sum_{\alpha\beta} |O_{\alpha\beta}|^2}$$

$$+ \frac{k_0^6 E_d}{160\pi\varepsilon_0 v_d \sum_{\alpha\beta} |M_{\alpha\beta}|^2} + \frac{k_0^8 E_d}{3780\pi\varepsilon_0 v_d \sum_{\alpha\beta\gamma} |O_{\alpha\beta\gamma}|^2},$$

$$I_{\text{inc}} = \left( \frac{\varepsilon_0 E_d}{\mu_0} \right)^{1/2} |E_{\text{inc}}|^2 / 2.$$
where \( \nu_0 = \frac{c}{\sqrt{\epsilon_d}} \) is the speed of light in the surrounding medium. Thus, the scattering cross-section \( \sigma_{\text{sca}} \) is presented as:

\[
\sigma_{\text{sca}} \approx \frac{k_0^4}{6\pi\epsilon_0 |E_{\text{inc}}|^2} \left| \mathbf{P} + \frac{ik_0\epsilon_d}{c} \mathbf{T} \right|^2 + \frac{k_0^4 \mu_0}{6\pi\epsilon_0 |E_{\text{inc}}|^2} \left| \mathbf{m} \right|^2
+ \frac{k_0^6 \epsilon_d}{720\pi\epsilon_0 |E_{\text{inc}}|^2} \sum |O_{sf}|^2 + \frac{k_0^6 \epsilon_d^2 \mu_0}{80\pi\epsilon_0 |E_{\text{inc}}|^2} \sum \left| M_{sf} \right|^2
+ \frac{k_0^6 \epsilon_d^2}{1890\pi\epsilon_0 |E_{\text{inc}}|^2} \sum \left| O_{sf} \right|^2.
\]

where \( k_0, \epsilon_0 \) and \( \epsilon_d \) denote the free-space wave number, vacuum permittivity, and relative dielectric permittivity of a surrounding medium is air (we consider \( \epsilon_d = 1 \)), respectively, \( \mu_0 \) is the vacuum magnetic permeability, \( c \) stands for the speed of light in vacuum, \( E_{\text{inc}} \) is the electric field amplitude of the incident light wave, and \( \mathbf{P} + \frac{ik_0\epsilon_d}{c} \mathbf{T} \) is a term including the interference of the electric dipole (ED) and toroidal dipole (TD) moments. Our approach can rigorously analyze the multimode decomposition in the scattering spectra of the Au–Si sliced nanorod.

The forward and backward scattering cross-sections of the nanoantenna can be determined by an integral of Poynting vector in the semi-space with the \( z \) coordinate > 0 and \( z \) coordinate < 0 as follows:

\[
C_{\text{sca,F}} = \int_{z>0} S_{\text{scat}} \cdot \hat{n} dA/I_{\text{inc}},
\]

\[
C_{\text{sca,B}} = \int_{z<0} S_{\text{scat}} \cdot \hat{n} dA/I_{\text{inc}}.
\]

An artificial boundary condition of the perfectly matched layer (PML) is added to the outer computational region to absorb radiation energy. The perfect electric conductor (PEC) adds a reflecting boundary condition to truncate the modeling domain. In addition, the Wave Equation, Electric 1 feature node link to the Materials feature node to obtain physical properties such as the relative permittivity constant that has been interpolated in the global function.
Figure 1 displays the schematic diagram of the Au–Si sliced nanorod. The height and radius of the Au–Si sliced nanorod are $h = 160\, \text{nm}$, $r_1 = 50\, \text{nm}$ and $r_2 = 50\, \text{nm}$, respectively. And the position of $z = 0$ has been indicated by point A. The incident light is a linearly polarized plane wave and the propagation direction of the incident light is along (frontal excitation) the cylinder axis. $H$ is the magnetic field, $E$ is the electric field, $K$ is the wave vector, and $H$, $E$, and $K$ correspond to the $x$-axis, $y$-axis, $z$-axis, respectively. The dielectric permittivity of silicon and gold are determined by Ref. [32] and Ref. [33].

## 3 Results and discussion

First, we investigate the scattering properties of an Au nanorod. The radius and height of the Au nanorod is $r = 50\, \text{nm}$ and $h = 160\, \text{nm}$. Figure 2 shows the normalized multimode contributions to the scattering cross-section of the Au nanorod. The resonant peak of the nanorod is explained by the multimode decomposition when the resonant contributions from different multimodes are tuned to overlap spectrally.

A broad resonant peak corresponding to wavelength of 552 nm is ascribed to the electric dipole (ED) resonance. Over the whole spectrum, ED plays a dominant role and the contributions of magnetic dipole (MD), toroidal dipole moment (TD), electric quadrupole moment (EQ), and magnetic quadrupole moment (MQ) are negligible.

Figure 4 Normalized multimode contributions to the scattering cross-section of the Au–Si sliced nanorod with $r_1 = r_2 = 50\, \text{nm}$, $h = 150\, \text{nm}$.

Figure 5 Normalized a MD moment, b ED moment, and c TD moment contributions to the scattering cross-section of the Au–Si sliced nanorod with different radii and $h = 160\, \text{nm}$.
The normalized forward scattering (FS), normalized backward scattering (BS), and the forward-to-backward ratio spectra (FS/BS ratio) are plotted in Fig. 3a. Forward and backward scatter can be determined by the Poynting vector in half space in the semi-space where \( z > 0 \) and \( z < 0 \). It is obvious that the maximum intensity of the FS/BS ratio appears at the wavelength of 338 nm and the corresponding intensity of FS/BS ratio is approximately 9.5. To demonstrate the scattering properties of Au nanorod, Fig. 3b, c shows the scattered field patterns of Au nanorod at the wavelength corresponding to the maximum of the FS/BS and the resonance of scattering cross-section, respectively. As is shown, at the wavelengths of \( \lambda = 337 \) nm and \( \lambda = 552 \) nm, the backward scattering is not completely suppressed, therefore, the individual Au nanorod can not reach the unidirectional forward scattering.

Figure 4 shows the normalized multimode contributions to the scattering cross-section of the Au–Si sliced nanorod with \( r_1 = r_2 = 50 \) nm and \( h = 160 \) nm. The refractive index of the surrounding medium is equal to 1. The resonance peaks of the scattering cross-section of the Au–Si sliced nanorod can be explained by multimode decomposition when the resonant contributions from different multimodes are tuned to overlap spectrally [34].

As is shown by the orange curve, it is clear that total scattering cross-section has a sharp peak at 480 nm, which has originated from the combination of the electric dipole, magnetic dipole and toroidal dipole resonances. There is one insignificant resonance peak at 451 nm which primarily arises from the electric dipoles. Moreover, the MD, ED and TD make significant contributions to the scattering cross-sections, while the separate contributions of the MQ and EQ terms are close to zero. Owing to the MD, ED and TD resonances, strong local magnetic field and electric field enhancements in the Au–Si sliced nanorod lead to novel scattering phenomena including vanishing backward scattering boding well for nanoantennas in nanoelectronics. In addition, contrast to Au nanorod, the spectrum becomes blue-shifted and narrower. It is attributed to the surface plasmon coupling when the noble metals are cooperated with semiconductors [35]. Thus, comparing with the normalized scattering cross-section of Au nanorod, several different multipolar moments are excited in Au–Si sliced nanorod.

The scattering properties of the Au–Si sliced nanorod are affected by the aspect ratios and they are adjusted by modulating only the radius of the Au–Si sliced nanorod from 30 nm to 70 nm at a fixed height of 160 nm. The aspect ratios of the Au–Si sliced nanorod are 5.33 (\( r_1 = r_2 = 30 \)), 4.0 (\( r_1 = r_2 = 40 \)), 3.2 (\( r_1 = r_2 = 50 \)), 2.6 (\( r_1 = r_2 = 60 \)) and 2.28 (\( r_1 = r_2 = 70 \)), respectively. Figure 5 shows the normalized contributions of the MD moment, TD moment, and ED moment to the scattering cross-section spectra of the Au–Si sliced nanorod with different radii and \( h = 160 \) nm. The different multimode contributions to the scattering cross-section of the Au–Si sliced nanorod can be tuned by simply adjusting the aspect ratio. The resonance spectra redshift as the radii are increased and the spectral distances between different multimode resonances peaks can be regulated by changing the nanoparticle aspect ratio. In addition, the resonance intensity of the MD, ED, and TD moments increases inversely with the aspect ratios and the contribution of the TD moment shown in Fig. 5c is smaller than those of the MD and ED moments as shown in Fig. 5a, b, respectively. The resonant wavelengths of \( r_1 = r_2 = 30 \) nm, \( r_1 = r_2 = 40 \) nm, \( r_1 = r_2 = 50 \) nm, \( r_1 = r_2 = 60 \) nm are correspondingly shorter than for \( r_1 = r_2 = 70 \) nm and the intensity of resonant peak is low, showing a large dependence of multimode modes on \( r \).

Figure 6 displays the normalized dependences of the magnetic field enhancement coefficients and the normalized electric field enhancement coefficients on the wavelength for the Au–Si sliced nanorod and Au nanorod with a radius of \( r_1 = r_2 = 50 \) nm, \( r = 50 \) nm and height of 160 nm in air.
As shown in Fig. 6a, we compare magnetic field enhancement coefficients of Au–Si sliced nanorod with the magnetic field enhancement coefficient of Au nanorod at the nanorod center. The maximum value of magnetic field enhancement coefficient for Au–Si sliced nanorod ratio can be up to 22.87 and is approximately 6 times larger than that of the Au nanorod. Due to the mismatched refractive index at the interface of Au and Si, the plasmon resonance that the particle would support inside a homogeneous medium is split, hence the field enhancement is larger in the case of Au–Si sliced nanorod as compared with Au nanorod [36]. In addition, the resonance and consequent enhancement of magnetic field always correspond to the resonance of different multimodes, and the resonance wavelength of magnetic field enhancement coefficient is 480 nm which is consistent with that of the total scattering cross-section. The enhancement coefficient can be enhanced by 22.87 times, giving rise to strong local magnetic field enhancement and providing a means of sensing on nanoscale [25]. Figure 6b shows normalized electric field enhancement coefficients on the wavelength. It is obvious that the electric field enhancement of the Au–Si sliced nanorod is larger than that of the Au nanorod. The maximum value of the electric field enhancement appears at 444 nm, which is almost consistent with the resonance wavelength for the ED in the Au–Si sliced nanorod shown in Fig. 4.

The electric field distribution profiles in the Au nanorod and Au–Si sliced nanorod at the scattering peaks of 552 nm and 480 nm are shown in Fig. 7. The red arrows show the circulating polarization density distributions. The electric field in the Au nanorod at wavelength of 552 nm symmetrically distributes around the Au nanorod, which is caused by electric dipole resonance. While, the electric field in Au–Si sliced nanorod inhomogeneously distributes around the silicon side of the Au–Si sliced nanorod. Due to the hybrid resonance modes, two cross-cuts of the displacement current loops on the silicon side of the Au–Si nanorod are generated.

Figure 8 shows the scattering properties of the Au–Si sliced nanorod with a radius of $r_1 = r_2 = 50$ nm and height of 160 nm in air. As is shown, the forward-to-backward spectra have two resonances in the visible region correspond to the wavelength of 435 nm and 514 nm. Owing to the inevitably destructive interference of different multimode moments, the maxima ratio of the FS/BS intensity occurring at 514 nm is approximately 14.19. Furthermore, the maximum intensity of the FS/BS ratio of Au–Si sliced nanorod is larger than that of Au nanorod, indicating that Au–Si sliced nanorod can provide high directivity in such case. The maximum value of the forward/backward scattering ratio of the Au–Si sliced nanorod is in the same

![Fig. 7](image1.jpg)

**Fig. 7** The electric field distribution for **a** Au nanorod and **b** Au–Si sliced nanorod at the scattering peaks

![Fig. 8](image2.jpg)

**Fig. 8** Spectra of forward/backward scattering ratios, normalized forward scattering and normalized backward scattering of the Au–Si sliced nanorod with $r_1 = r_2 = 50$ nm and $h = 160$ nm
magnitude with the those values reported in Ref. [24, 37, 38], and the Au–Si sliced nanorod suppresses the backward scattering and enhances the forward scattering at spectral wavelength.

To explicitly demonstrate backscattering suppression, Fig. 9 depicts the contours of the angular distributions of the scattering intensity in the far scattering field at multimode wavelengths of the forward-to-backward ratios and normalized scattering cross-section of Au–Si sliced nanorod. The angles of 90° and 270° in Fig. 9 represent the forward scattering and backward scattering, respectively. Backward scattering is substantially suppressed and scattering in the forward direction is dramatically enhanced. In addition, the radiated far fields are in phase with forward scattering and no backward scattering is obtained which is due to the destructive interference between the MD, ED and TD multipolar resonant moments. Hence, by overlapping the resonant contributions of several different multipolar moments, multiple unidirectional forward scattering can be modulated. Furthermore, compared with angular distributions of Au nanorod, no backscattering is obtained between these multipolar resonant moments in the case of Au–Si sliced nanorod, indicating that the multiple unidirectional forward scattering can be achieved in the proposed Au–Si sliced nanorod.

4 Conclusion

The Au–Si sliced nanorod with $r_1 = r_2 = 50$ nm and $h = 160$ nm exhibits two resonances in the visible region and is investigated by the multimode decomposition method. The resonances excited by the Au–Si sliced nanorod are stem from the different multipolar moment modes. The ability of the nanorod to suppress backward light scattering and simultaneously enhance forward light scattering at multiple wavelength band can be explained by the constructive interference between different multimode resonances generated by the multimodes. The Au–Si sliced nanorod has potential as high-performance nanoantennas and offers a feasible strategy to tailor directional scattering and engineer light flow.

Acknowledgements This work was supported by Natural Science Foundation of Heilongjiang Province (Grant no. E2017010, E2016007), Northeast petroleum university “national fund” cultivation...
funds (Grant no. 2017PYZL-08), Northeast Petroleum University Innovation Foundation For Postgraduate (Grant no. JYCX_CX09_2018) as well as Hong Kong Research Grants Council (RGC) General Research Funds (GRF) Nos. CityU 11301215 and 11205617.

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