A silicon trimer is explored to tailor unidirectional forward scattering at multiple wavelengths in the near-infrared region with low loss using theoretical calculations and numerical simulations, which leads to the dramatic enhancement in unidirectional forward scattering and suppression of backward scattering. The higher moments in the trimer can be properly excited and balanced by breaking the symmetry of the trimer. The generalized Kerker conditions at two different wavelengths can be achieved in the trimer to further improve the scattering directivity. Our results provide insights into future development of all-dielectric low-loss nanoantennas in the near-infrared region.

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1. INTRODUCTION

Light scattering of small particles has been the focus of many studies in optical communication, biophysics, astrophysics, and materials science [1–3]. Effective control of optical radiation at the sub-wavelength scale, e.g., suppression of unwanted backward scattering (BS) and enhanced directed forward scattering (FS), is one of the critical issues in research fields related to particle scattering and plays an important role in applications such as sensors [4–7], nanoantennas [8,9], photovoltaic devices [10], and light-emitting devices [11]. The optical properties of individual structures with a regular shape in these applications have also been extensively studied, e.g., cylinders and disks [12,13], spherical particles [14], nanoblocks [15], and rectangular nanowires [16,17]. It has been studied that in these structures, the electric dipole (ED) and magnetic dipole (MD) resonances are the two basic modes of easy excitation, and the particle supports the same magnitude of overlapping electric and magnetic multipoles would not scatter backward [1,18].

In recent years, interfering multipoles that can cause unidirectional scattering have been extended from dipoles to higher-order multipoles and coupling between different multimode resonances [19]. By means of spectral overlap, Kerker-type scattering shows the superior directional scattering capability and is widely used in ultra-directional FS of dielectrics and metallic nanoantennas. Kerker theoretically proposes FS with super-directional enhancement with the superior directional scattering capability through spectral overlap. Therefore, Kerker-type scattering of dielectric and metal nanoantennas has been explored [20]. In addition, the experimental samples of all-dielectric trimer nanoantennas have been fabricated by a cost-effective chemical method [21], highly precise pick-and-place technique [22], and laser printing method, exhibiting great potential applications in solar cells, lighting instruments, directional scattering, and surface-enhanced spectroscopies [23,24]. More recently, a laser printing method has successfully been used to fabricate silicon nanospheres due to the advantages of a single-step process, high reproducibility, and accurate space arrangement of the nanoparticles. The different inter-particle distances of 5–375 nm can be obtained [25,26]. Compared with dielectric nanoantennas with high refractive indices and low loss, metal nanoparticles have inherent limitations. Since the dipole mode is a surface mode, the resonant characteristics are sensitive to the surroundings, and dielectric loss is high in the visible and near-infrared regions. However, multiple unidirectional FS of a trimer with dielectric materials in the near-infrared region has not been systematically studied.

Herein, we propose a novel all-dielectric trimer nano-antenna that can support multiple resonance modes of the MD, ED, and electric quadrupole (EQ) moments to achieve unidirectional FS in the near-infrared region at multiple wavelengths numerically. Toroidal dipole (TD) moment is neglected due to the fact that TD is one of the expansion terms of the
2. SIMULATION MODEL

The multipole decomposition method is used to analyze the scattering characteristics when the contributions from different multipoles to the silicon trimer are tuned to overlap in the spectrum [30]. The multipole expansion in Cartesian coordinates is shown below. It is derived from Taylor expansion of the vector potential. Equations (1)–(5) are the formulas for the contribution of the ED moment $P$, EQ moment $Q'$, MD moment $M$, and magnetic quadrupole (MQ) moment $Q''$, respectively [31]:

$$P = \int P(r')dr', \quad (1)$$

$$Q' = 3 \int [r'P(r') + P(r')r']dr', \quad (2)$$

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

$$Q'' = -\frac{2i\omega}{3} \int [r' \times P(r')]r'dr', \quad (4)$$

where $P(r')$ is the polarization generated by the incident light wave in scattering, and $r'$ is the radius vector of the volume element in the scattering medium. The total radiation energy of the multipolar moment can be presented as [32–36]

$$I = \frac{2\omega^4}{3c^2} |P|^2 + \frac{2\omega^4}{3c^2} |M|^2 + \frac{\omega^6}{20c^3} |Q'|^2 + \frac{\omega^6}{20c^3} |Q''|^2. \quad (5)$$

In the formula, $\omega$ is the angular frequency, $\varepsilon_0$ denotes the dielectric constant in vacuum, and $c$ is the speed of light for the vacuum. The scattering cross section $C_{sca}$ can be expressed as the ratio of the radiant energy $I$ to the energy of the incident light wave $I_{inc}$, and the expression is

$$C_{sca} = \frac{I}{I_{inc}}. \quad (6)$$

The silicon trimer is schematically shown in Fig. 1, the three spheres with a radius of $R = 170$ nm and the spacing $d$. Point A and point B are at the center of the spacing $d$. In the simulation, the incident light is a linearly polarized plane wave, and the propagation direction of the incident light is along the $x$ axis with linear polarization along the $y$ axis. The dielectric permittivity of silicon is obtained from the experimental data of Aspnes and Studna, and the background medium is assumed to be air (refractive index $n = 1$) [37].

3. RESULTS AND DISCUSSION

Figure 2 shows the scattering cross section of the silicon trimer nanoparticles with a radius of $R = 170$ nm, and the gap $d$ is 5 nm between the nanoparticles. The numerical calculation is performed using the finite element method (FEM) based on COMSOL Multiphysics, and the method of multipolar decomposition is implemented to explain the resonance peaks of the silicon trimer [38]. The positions of the two pronounced resonant peaks in the total scattering spectrum (Sum Scat, yellow line) are in the near infrared region corresponding to wavelengths of 1102 nm and 1336 nm. The resonances arise from the combined contributions of the MD moment (blue line), ED moment (green line), and EQ (magenta line). When the wavelength is 1102 nm, a sharp peak is generated due to ED, MD, and EQ resonance, and the second peak at 1336 nm can be ascribed to ED and MD resonance. Compared with the scattering peaks caused by the combined contributions of different multipole moments, two resonant peaks in the scattering spectrum of the symmetric trimer nanostructure in a gold film are due to antibonding and bonding plasmon resonant modes [39], respectively. It is worth noting that MD and ED are in a dominant position across the spectrum, but the contribution of the MQ (red line) to the scattering cross section is approximately zero over the entire spectrum. Owing to the simultaneous appearance of ED, MD, and MQ at 1336 nm, pronounced enhancement of the total scattering cross section can be seen, and this is known as superscattering [40,41]. In order to verify the correctness of the FEM, the normalized scattering cross sections of the spherical objects with small particle gap are calculated by using Mie method and FEM, as shown in Fig. 2(b). The results obtained by the two methods have good consistency, especially in that the position and trend of the main peak are the same, confirming accuracy and efficiency of the FEM.
It is noted that there are slight differences between the two curves due to the different calculation principles and the total number of grids, and the calculation of the post-processing electromagnetic field may lead to some numerical errors.

Figure 3(a) presents the normalized scattering properties of the FS to BS (FS/BS) ratio for the silicon trimer. The integral of Poynting’s vector in the semi-space with \( x > 0 \) can be defined as FS and \( x < 0 \) can be defined as BS. The two distinct peaks of the FS/BS ratio spectrum are located at \( \lambda = 0.136 \) nm and \( \lambda = 0.136 \) nm, which are identical to the two intersections in the \( K \) curve as shown in Fig. 3(b). It can be observed that owing to destructive interference of the multipolar moments of MD, ED, and EQ, with simultaneous spectral overlap and comparable strength, BS is substantially suppressed [42]. At the wavelength of 1300 nm, the maximum ratio of the FS/BS intensity is approximately 16.3, indicating that forward direction scattering is enhanced and high directivity is achieved.

According to the study on the hypothetic magneto dielectric particles conducted by Kerker et al. and the generalized Kerker condition for highly directive nanoantennas, the radiated far field of a nanoantenna can be described as [43]

\[
E_{\text{inc}}(r) = \frac{k_0^2}{4\pi\varepsilon_0 r} e^{ik_0 r} \left\{ \hat{n} \times (D \times \hat{n}) + \frac{(m \times \hat{n})}{c} + \frac{ik_0}{6} \hat{n} \times (Q \cdot \hat{n}) + \cdots \right\},
\]

where the MD moment is \( m \), the term \( D \) can be defined as ED, \( Q \) is EQ moment, \( k_0 \) is the free-space wavenumber, and \( \varepsilon_d \) represents the relative permittivity of the surrounding medium equal to 1. The backward radar scattering cross section of the nanoantenna can be defined as [18]

\[
\sigma_{\text{BW}} = \frac{k_0^4}{4\pi|E_{\text{inc}}|^2} \left( p_y - \frac{\sqrt{E_d}}{c} m_z + \frac{ik_0}{6} Q_{xy} \right),
\]

where \( |E_{\text{inc}}| \) is the modulus of the incident electric field. It is well known from the so-called generalized Kerker condition that if zero BS occurs, the following Kerker condition must be fulfilled:

\[
p_y - \frac{\sqrt{E_d}}{c} m_z + \frac{ik_0}{6} Q_{xy} = 0.
\]

To analyze the underlying scattering mechanism of the silicon trimer, the dependence of the real and imaginary components of Eq. (10) on the wavelength are sketched in Fig. 3(b). For convenience, it is defined as
The generalized Kerker condition at the maximum of ratio is fulfilled. $K$ is close to zero (both the real and imaginary parts) indicating substantial attenuation of BS and significant enhancement of FS. Moreover, the generalized Kerker effect relies on the interference between multipoles of different types and orders [44].

To compare the scattering properties of a silicon trimer with a typical metallic system, we investigate the multipole contributions to the scattering cross section of a gold trimer in Fig. 4(a). The structure of Fig. 4 is the same as that in Fig. 2 with $R = 170$ nm and $d = 5$ nm. The refractive index of the surrounding medium is equal to 1. As shown in Fig. 4(a), only one resonance is visible at $\lambda = 1,140$ nm in the scattering cross section, which corresponds to the contribution of ED resonance. Except for the ED moment, the contribution from other multipole moments in the total scattering efficiency spectrum is almost negligible. To clarify the scattering characteristics of the gold trimer, Fig. 4(b) displays the FS/BS ratio and the corresponding 3D scattering pattern at the maximum of ratio is shown in the inset. The maximum value of the FS/BS curve is 2.45, proving that the gold trimer does not reach unidirectionality, and the 3D far-field image in the inset of Fig. 4(b) confirms it. BS of the gold trimer is not completely suppressed at the resonant wavelength of $\lambda = 851$ nm, and the dependence of the real and imaginary components of $K$ on the wavelength of the gold trimer is presented in Fig. 4(c), which clarifies that the gold trimer does not satisfy the Kerker-type condition. Figure 4(d) shows a comparison of the forward to backward radar scattering cross sections for the gold trimer and silicon trimer. Two distinct resonances can be seen from the silicon trimer compared with the unnoticeable resonant wavelength for the gold trimer in the near-infrared region.

We further investigate the effects of the trimers with different configurations on the multipole scattering cross sections and unidirectional scattering. The radius of the trimer is $R = 170$ nm, and the distance between each sphere is 5 nm. To elucidate the physical mechanism of unidirectional scattering of the equilateral triangle structure, the scattering cross sections of multipolar modes is given in Fig. 5(a). As shown in the inset in Fig. 5(a), the trimer is adjusted to be an equilateral triangle structure, the most symmetrical structure of a trimer being degenerate [45]. Compared to the trimer in Fig. 1, the magnitude and bandwidth of the multipolar scattering cross section of the equilateral triangle trimer is reduced significantly. In this system, three types of multipole moments are efficiently excited. Because of the combined contributions of MD and ED, a sharp resonant peak is visible at $\lambda = 1,045$ nm. Figure 5(b) presents the FS/BS ratio and corresponding 3D scattering pattern versus the resonant wavelength of the equilateral triangle trimer. At $\lambda = 823$ nm and $\lambda = 1,319$ nm, backward direction is suppressed because of destructive far-field interference [46].

With a gradually increasing vertex angle, the symmetry is broken, and the configuration changes from an equilateral triangle to a linear-chain trimer, as shown in the inset of Fig. 6(a). By summing the contributions of all the multipolar moments, Fig. 6(a) shows the scattering cross section of the silicon trimer with the chain structure versus the incident wavelength. The parameter of the trimer is 170 nm, and the spacing between the trimers is 5 nm.
each sphere is 5 nm. The index of the surrounding medium is also 1. Owing to interference of MD and ED, sharp and broadband resonances can be seen at $\lambda = 913$ nm and $\lambda = 1,253$ nm, respectively. It is noted that the contribution of MQ and EQ is negligible over the whole spectrum for this chain structure. The FS/BS ratio spectrum is shown in Fig. 6(b), and the maximum of the FS/BS intensity ratio is approximately 9.54. The 3D far-field scattering pattern of the two peaks at $\lambda = 823$ and $\lambda = 1,208$ nm is also given in the inset of Fig. 6(b), and it indicates that forward scattering is enhanced at the resonant wavelength of the FS/BS ratio. Comparing the scattering properties of the trimer in Fig. 1 to the equilateral triangle trimer, the symmetry damage in the nanostructure can introduce high-order multipoles that do not exist in a symmetrical configuration.

By varying the radius of the trimer and width of the gap, Fig. 7 systematically reveals the influence of the change in the radius and gap width on the FS/BS ratio and electric field enhancement. As shown in Fig. 7(a), the intensity of the FS/BS ratio in one of the trimers does not change with different radii, demonstrating that unidirectional scattering has little dependence on the size distribution. It benefits from the oligomer structure and achieving unidirectional effects. However, as the radius decreases from 170 nm to 150 nm, resonances blue shifts to the visible region. It should be pointed out that the gaps between different trimers are the same and therefore, to keep the resonances in the near-infrared range of the spectrum, each sphere has a radius of 170 nm. Figure 7(b) displays the FS/BS ratio calculated with the same radius of the trimer of 170 nm and considering different gap widths. Although the increase in the gap has a slight influence on the maximum value of the FS/BS ratio, there is almost no difference in the far-field scattering characteristics, as evidenced by the far-field 3D plot of the insets in Fig. 7(b). Furthermore, Figs. 7(c)–7(f) show the near-field enhancement of the electric field for different radii and gaps at the positions labeled as point A and point B, respectively. Figures 7(c) and 7(d) show that the near-field enhancement of the trimer having a radius of 170 nm is much larger than that of 150 nm and 160 nm at both point A and point B. The near-field enhancement characteristic for a trimer with a gap of 5 nm is also much larger than the gaps of 0 nm and 10 nm, as shown in Figs. 7(e) and 7(f).

Our calculations show that when the radius and gap of the trimer are 170 nm and 5 nm, intense localized electric near fields occur in the gap of the dielectric trimer, and the electric field enhancement at point A reaches a maximum of around 71 at the peak. The large field enhancement effect at the gap is an attractive property that can improve the Raman scattering signal of molecules effectively [47].

To obtain more physical insights into unidirectional scattering, Fig. 8 shows the near-field distribution on the $xoz$ plane of the electric and magnetic fields at the resonant peaks (816 nm, 1102 nm, and 1300 nm), corresponding to the resonant peaks of the scattering cross section and FS/BS ratio. The color map reveals the total electric or magnetic field intensity, and the white arrow indicates the field direction. Figures 8(a)–8(c) show that the electric field is significantly enhanced in the gap region of the trimer and electric “hottest spots” appear at the multipolar wavelength. A circular displacement current can be seen inside the trimer, and unlike the conduction current in metals with free electrons, the displacement current in the dielectrics is derived from oscillation of bounded electrons due to the field penetration and phase delay effects in the dielectric particles [48–50]. Meanwhile, bright hot spots with highly enhanced magnetic localized fields inside the trimer are indicated in Figs. 8(d)–8(f). The simulation results show that the magnetic field enhancement of the spheres in the trimer does not reach the maximum at the same time, and
the magnetic hot spots split into two at one resonant peak of the FS/BS ratio.

Figure 9 shows the surface charge distribution corresponding to the resonance frequencies in Fig. 8. The induced charges are distributed on the surface and have substantially opposite signs at the gap of the trimer. The red and blue colors indicate positive and negative charges, respectively. The charge distribution at 816 nm in Fig. 9(a) stands for quadrupole resonance resulting from the interference between the multipolar dipole of MD. However, the separation between positive and negative charges is not obvious [51]. When the wavelength is 1102 nm and 1300 nm, the charge distribution is dipolar due to the influence between each nanosphere in the trimer. The boundary between the positive and negative charges appears spatially distorted. As the strong electrostatic field generated by a high density of positive and negative charges on either side of the center sphere in Figs. 9(b) and 9(c) weakens the magnetic resonance energy, the responses to the magnetic field of the side spheres and sphere in the center in Figs. 9(b) and 9(c) are not synchronized [52].

Figure 10 presents the angular distributions of the scattering intensity in the far field and corresponding 3D scattering pattern at the resonant wavelengths of the FS/BS ratio to give an explicit demonstration of BS suppression. Herein, the full-width at half-maximum (FWHM) is defined as the main lobe angular beam width \( \alpha \) to describe the directivity of the primary scattering lobes. Angle 90° and angle 270° represent the forward and backward direction, respectively. BS is substantially suppressed, and FS is significantly enhanced at \( \lambda = 816 \text{ nm} \) and \( \lambda = 1300 \text{ nm} \). Because of destructive interference between different multipolar resonant moments in Fig. 2, the angular beam width in Fig. 10(a) is narrowed to 59°, indicating ultra-directional FS as a result of the equal magnitude scattering contribution from MD. The corresponding 3D scattering pattern is shown in Fig. 10(c). It should be noted that the additional side scatter lobes originate from the complex interaction between the dipole and quadrupole electrical and magnetic resonance with different amplitudes [53]. Figure 10(b) shows the 2D scattering patterns calculated at \( \lambda = 1300 \text{ nm} \), confirming that most of the scattering energy radiates into the forward hemisphere. BS is suppressed significantly, and the angular beam width is approximately 87°.

4. CONCLUSION

Unidirectional scattering derived from coupling between different multimode resonances of the silicon trimer is investigated by the multipole decomposition method. Depending on constructive interference among MD, ED, and MQ, unidirectional FS can be achieved at multiple wavelengths, and the generalized Kerker condition can be satisfied in the near-infrared regimes. The near-field enhancement property is also achieved, boding well for application of surface-enhanced Raman scattering. The symmetry breaking of the trimer has a large impact on excitation of higher-order multipoles, leading to enhanced directionality. Our study on unidirectional scattering provides insights into future development of novel nanoantennas, bio-sensors, and photovoltaic devices.

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