Enhanced light absorption of silicon in the near-infrared band by designed gold nanostructures*

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A scheme to enhance near-infrared band absorption of a Si nanoparticle by placing the Si nanoparticle into a designed gold nanostructure is proposed. Three-dimensional (3D) finite-difference time-domain simulations are employed to calculate the absorption spectrum of the Si nanostructure and maximize it by generating alternate designs. The results show that in the near-infrared region over 700 nm, the absorption of a pure Si nanoparticle is very low, but when the same nanoparticle is placed within an optimally designed gold nanostructure, its absorption cross section can be enhanced by more than two orders of magnitude in the near-infrared band.

Keywords: surface plasmon resonance, near-infrared, silicon absorption, finite-difference time-domain optimization

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1. Introduction

Silicon (Si) is the second most abundant element and comprises 25% of the Earth's crust. The properties of silicon nanoparticles have recently received considerable attention in plenty of areas. The wide applications of silicon include photodetectors,[1] concrete,[2] alloys,[3,4] electronics,[5] biology,[6,7] and so on. Because of the wide technology base (ASIC's, diodes, and detectors[1]) of silicon, which has for example helped to spawn the use of pixel detectors (hybrids, CCD's, CMOS detectors[8]) for truly two-dimensional applications, it has been the best choice in tracking devices.[9]

Surface plasmon polaritons (SPPs) are surface electromagnetic waves that propagate on the interface between metal and dielectric with their energy strongly confined at the interface. They are induced by incident light coupled to the collective oscillation of electron gas in metal. SPPs play a key role in many applications due to their relatively long propagation distance and strong confinement of light energy to the surface.[10] These unique properties can be used in a wide range of fields, including holography,[11] chemical and biochemical sensors,[12] solar cells,[13] lasing spasers,[14] surface-enhanced nonlinear mixers,[15] cancer cell treatment,[16] antenna[17,18] applications, and so on.

Optical antennae are nanostructures that can efficiently convert freely propagating optical radiation into localized energy, and *vice versa*.[19] They enable the control and manipulation of optical fields at the nanometer scale and hold promise for enhancing the performance and efficiency of photodetection,[20,21] light emission,[22,23] and sensing.[24]

Surface plasmon resonance can occur when light interacts with metal nanoparticles and nanostructures, which could produce light-harvesting effects. Optical antennae made from plasmonic materials can take advantage of the surface plasmon resonance effect to improve significantly their performance and efficiency at selected frequencies, an attribute that also holds promise for biological sensing and detection.[25–27] As the bandgap of Si is 1.12 eV, it has the disadvantage that it is only weakly absorptive for near-infrared radiations, and it exhibits large dark currents either before or after irradiation, which will reduce the sensitivity.[1] To improve the responsive efficiency of a Si photodetector, in this paper, we focus our attention on taking advantage of surface plasmon resonance in increasing the absorption of a Si nanoparticle in the near-infrared region. Some image intensifiers[28] are very sensitive to this area of the spectrum, for example night vision devices, including night vision goggles.[29]

We will use the three-dimensional (3D) finite-difference time-domain (FDTD) method[30,31] to investigate the optical properties of Si brought into a designed gold nano-antenna structure and compare them to the case of a pure Si nanoparticle. The results show that the absorption efficiency of a Si nanoparticle can be enhanced by more than two orders of magnitude when it is embedded within an appropriately designed gold nano-antenna structure.

2. Results and discussion

The photodetection performance of silicon nanoparticles can be well evaluated by their absorption cross section. The absorption cross section area is defined as

$$\sigma_{\rm abs}(\omega) = \frac{P_{\rm abs}(\omega)}{I_{\rm inc}(\omega)},$$

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where P_{abs} is total power absorbed by the Si particle, I_{inc} is the incident intensity. To achieve this important parameter, we first calculate the absorption cross section of pure Si via the 3D FDTD method. To calculate the total absorption power, we enclose an artificial surface surrounding the Si particle, for instance a spherical or cubic box surface, then calculate the electromagnetic energy power going inwards into the surface P_{in} and the electromagnetic energy power radiating outwards out of the surface P_{out}. According to the energy conservation principle, the absorption power is given by $P_{abs} = P_{in} - P_{out}$. Note that by adopting such a procedure, we have completely excluded the possible contribution of metal nanostructures adjacent to the Si particle. According to the optical constants given in Palik,[32] by doing linear interpolation over the data, we get the dispersion data of Si, and the complex refractive index of Si as a function of wavelength is plotted in Fig. 1. From the dispersion curve, we can see that the imaginary part of the refractive index in the near-infrared band is very small, all less than 0.01. This means that the light absorption of Si in that frequency band is very weak. This will greatly limit the absorption efficiency of Si and reduce the application of Si in near-infrared photodetectors. In our calculation, the maximum mesh step is 5 nm, and the model used in the simulation is a solid cubic nanoparticle with side length of 120 nm, as schematically illustrated in Fig. 2(a). The edges of Si are parallel to the x, y, and z axes, so we choose the center of the Si particle as the origin of coordinates. The incident light propagates along the z axis and the polarization direction is along the x axis. The absorption cross section of the pure Si nanoparticle is shown in Fig. 2(c) with a black line. From Fig. 2(c), we can find that in the near-infrared region over 700 nm, the absorption cross section of pure Si nanoparticle is very low, which is about 10^{-5} μm^2. The absorption efficiency, which is the ratio of absorption cross section over the geometric cross section area, 0.0144 μm^2, is on the order of 10^{-3}, meaning a very low level of absorption efficiency of Si material at near-infrared bands.

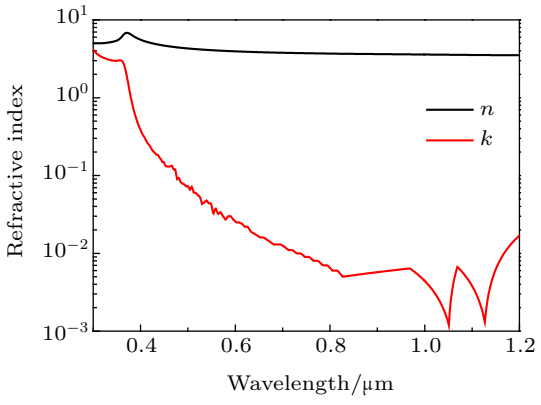


Fig. 1. (color online) The complex refractive index of Si in logarithmic scale as a function of wavelength.

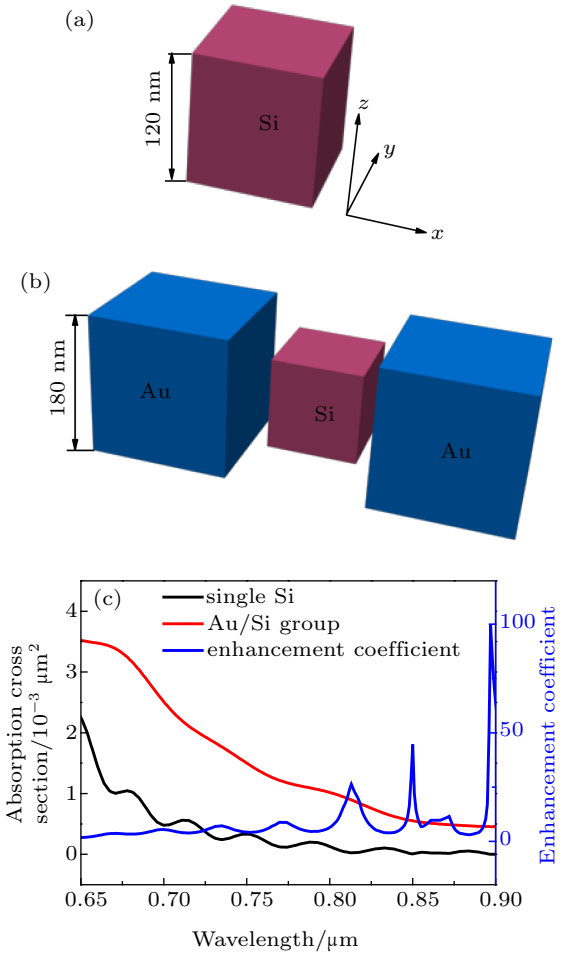


Fig. 2. (color online) (a) Model of Si nanoparticle used in the simulation. The side length of cubic Si nanoparticle is 120 nm. (b) Model of the Au/Si group used in the simulation, the sizes of Si and Au cubic nanoparticles are 120 nm and 180 nm, respectively. The distance between Si and Au nanoparticles is 4 nm. (c) Contrast between absorption spectrum of pure Si particle (120 nm) and Au/Si particles (Si 120 nm, Au 180 nm), and the corresponding enhancement coefficient of Si absorption cross section.

To improve the absorption efficiency of the same Si nanoparticle, we turn to consider surface plasmon resonance because it is well known that this effect could produce light-harvesting effects when light interacts with metal nanoparticles and nanoparticles or nanostructures. Here we propose a scheme to enhance near-infrared band absorption of an Si nanoparticle by introducing Au particles. To show whether it is the case, a model of the Au/Si group is set up as shown in Fig. 2(b): one Si particle is placed in the middle of two Au particles. The Au particle is also a cube and the edge lengths of Si and Au are 120 nm and 180 nm, respectively. The origin of coordinates is still chosen at the center of the Si particle. The distance between Si and Au is 4 nm in our simulation and the maximum mesh step is 5 nm. In Fig. 2(c), we compare the absorption cross section spectrum of pure Si (the black line) with that of an Au/Si particle group (the red line). Under the influence of Au nanoparticles, the absorption cross section of Si increases obviously in the near-infrared region. To describe the enhanced absorption effect more quantitatively, we define

the relative magnification factor of the absorption cross section of an embedded Si nanoparticle divided by that of a pure Si nanoparticle as enhancement coefficient. The results are shown in Fig. 2(c) with a blue line. For some wavelengths, the enhanced absorption effect is great. For example, the absorption cross section of pure Si and that of an Au/Si particle group at a wavelength of 815 nm are 2.8×10^{-5} μm^2 and 6.5×10^{-4} μm^2, respectively, so the enhancement coefficient is 23. And the enhancement coefficient is 45 at 850 nm and 57 at 960 nm.

To obtain more clarified physical pictures, we calculate the electric field intensity patterns for (a) a pure Si particle (120 nm) at a wavelength of 850 nm and (b) the Au/Si particles (Si 120 nm, Au 180 nm) at a wavelength of 850 nm as shown in Fig. 3. The maximum field intensity in panel (b) is almost 39, while in panel (a) the maximum is only 8. In Fig. 3, we can see obviously that when the incident light shines on the Au/Si particles, the light is harvested and the field is greatly enhanced within the gap of the Au particles at the wavelength of 850 nm compared with the situation of a pure Si particle. Hence, the intensity of near-infrared light that the Si particle receives is much larger than the incident light intensity, and hereby, of course, the effective absorption cross section of the Si particle has been greatly improved. To put it in a nutshell, the Au particles here act as an antenna for near-infrared light.

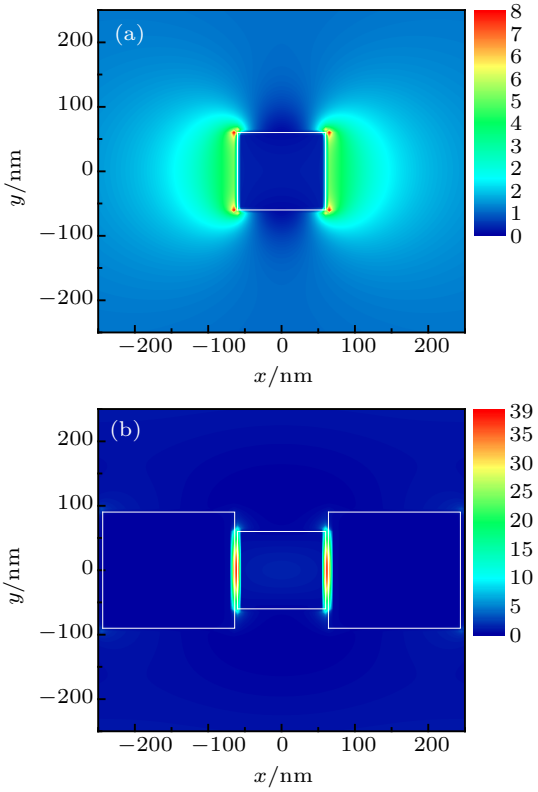


Fig. 3. (color online) Calculated electric field intensity patterns for (a) a pure Si particle (120 nm) and (b) the Au/Si particles (Si 120 nm, Au 180 nm) at the wavelength of 850 nm. The field intensity is in units of the incident field intensity.

The above discussion has demonstrated that taking advantage of the scattering and local field enhancement features of surface plasmon resonance can improve the effective absorption cross section of an Si particle, but the enhanced absorption effect is not too high. In contrast to 2D planar nanostructures, 3D nanostructures can produce more "hotspots".[33–35] In these hot spots, the local electromagnetic field obtains a strong enhancement, which is conducive to enlarging the interaction of light and matter. This opens our mind to come up with an effective method to improve the pure Si absorption cross section in the near-infrared region, that is, to find an appropriate 3D Au nanostructure which has prominent local field enhancement. The geometry of the successfully designed Au nanostructure is shown in Fig. 4(a) and Fig. 4(b). The Si nanoparticle is embedded in a rectangular slot, which is located at the center of the Au nanostructure, which is a bit bigger than the Si particle in each edge length. It looks like the Si is surrounded by an Au wall. The height and the thickness of the wall are h and t, respectively, and the height and the thickness of the slot is Δh and Δt. The origin of coordinates is set at the center of the Si particle, and the bottom surface of the Si nanocube of the slot is 5 nm upon the bottom of the slot. The x and y axes are parallel to the square edges of the Au rectangle.

We employ the 3D FDTD optimization method that is supported by the software package[36–38] to find the best geometric parameters which can maximize the absorption cross section of Si material. Optimization is a powerful feature of the FDTD software package that allows users to automate the process of finding desirable parameter values by running a large number of simulations. The optimization project allows users to use built-in algorithms as well as define their own optimization algorithms. In our calculation, we choose the particle swarm optimization (PSO) algorithm. PSO is a population-based stochastic optimization technique, inspired by the social behavior of flocks of birds or schools of fish,[39,40] and it has been widely used for various kinds of design optimization problems[40] including nanophotonic design.[41–43] In the optimization, the result is set as the maximum of the absorption cross section of the Si particle. The edge length of Si nanocube is 120 nm. The generation size (number of children per generation) for this optimization project is 10. That means during the procedure of optimization, we get 102 groups of parameters. We obtain a group of parameters from the 100 groups at last that can maximize the absorption cross section spectrum of the Si nanoparticle.

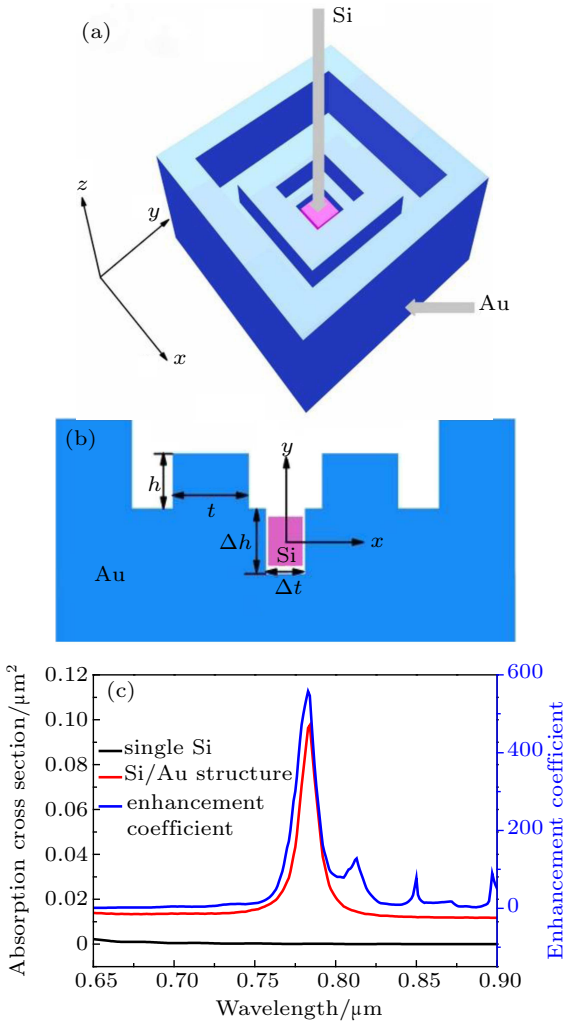


Fig. 4. (color online) (a) 3D view panel and (b) lateral view of the designed 3D Au nano-antenna embedded with an Si nanoparticle. (c) Comparison between absorption spectrum of pure Si particle (120 nm) and optimized Au/Si structure with parameters $h = 100$ nm, $t = 265$ nm, $\Delta h = 130$ nm, and $\Delta t = 140$ nm.

For discussing the influence of the factor of the designed Au nanostructure and making sure we have got what we want, we simulate four other structures determined by four parameters plotted in Fig. 4(b) and named h, t, Δh, Δt. Each time we change a parameter, the other three parameters remain unchanged. The absorption cross section of Si with five different parameters is plotted in Fig. 5(a). The first group of optimization is what we want, and the parameters will maximize the absorption cross section of the Si nanoparticle. Choose parameters as $h = 100$ nm, $t = 265$ nm, $\Delta h = 130$ nm, and $\Delta t = 140$ nm. The absorption cross section of the Si nanoparticle is shown in Fig. 4(c) with a red line for the optimized Au nano-antenna structure. It can be clearly seen that the absorption cross section of Si significantly increases, and has its maximum value of about 0.1 μm^2 located near 784 nm. For comparison, the absorption cross section of pure Si at 784 nm is just 1.8×10^{-4} μm^2. In addition, from the blue line in Fig. 4(c), we can see that when placed within the designed Au nanostructure, the absorption cross section of Si particle can be enhanced by more than two orders of magnitude in the near-infrared band. From Fig. 5(a), we can see that when the four parameters change a little, the maximum decreases as well as the enhancement coefficient, as plotted in Fig. 5(b). Thus it is clear that we have obtained the maximum absorption.

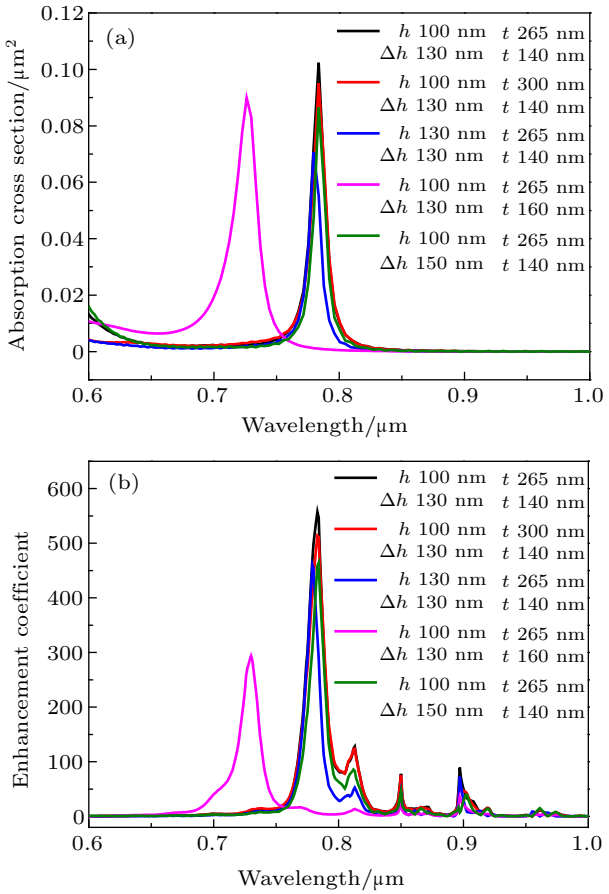


Fig. 5. (color online) (a) Absorption spectra and (b) the corresponding enhancement coefficients of five nano-antenna structures with parameters as noted.

The discussion above shows us the influence of the geometric factor of the designed Au nanostructure on the absorption properties; the discussion below will exhibit the great influence of the geometric parameters of Si nanoparticles on the absorption cross section of an Si particle. To see this, we have changed the size of the Si nanocube from 90 nm to 130 nm with other parameters of the Au nanostructure unchanged. The calculated absorption cross section spectra of embedded Si nanocubes with different sizes are plotted in Fig. 6(a). From these curves we can find that Si nanocubes with a larger edge length will lead to a much larger red shift of absorption spectrum. But the maximum enhancement coefficient of Si particle, as plotted in Fig. 6(b), appears at the 120-nm edge length and a wavelength of 784 nm. Moreover, when the size of the Si particle becomes too large, the confinement capability of the near-infrared optical field becomes lower in the large-size slot of the designed structure.[17]

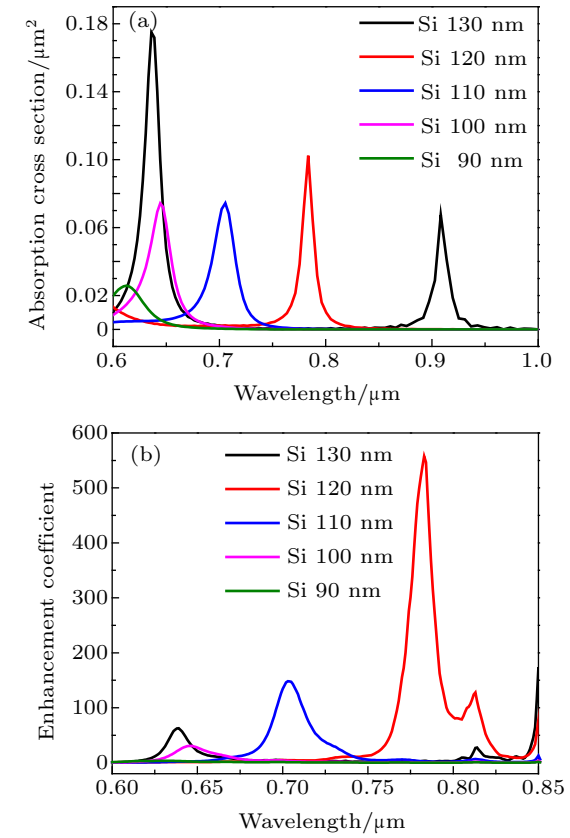


Fig. 6. (color online) (a) Absorption cross section of embedded Si nanocubes with different sizes and (b) the corresponding enhancement coefficient.

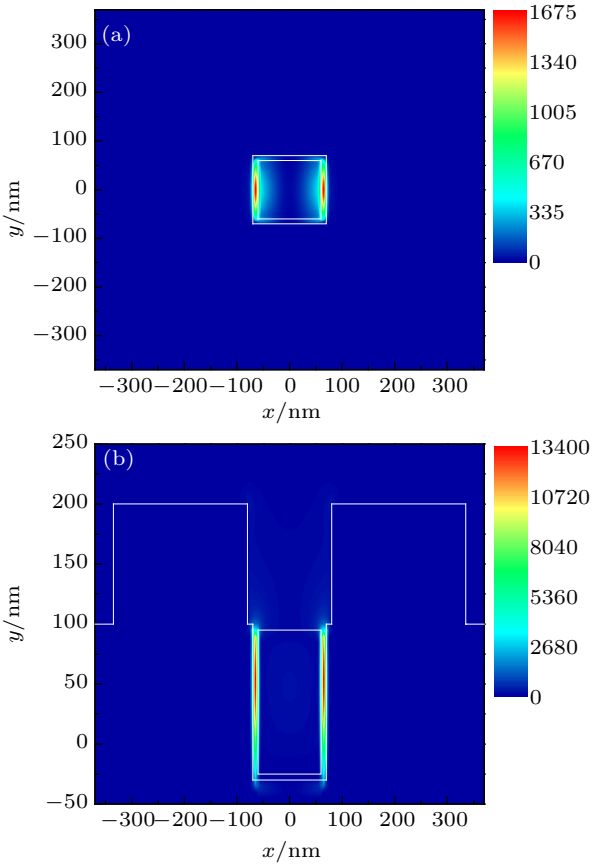


Fig. 7. (color online) Calculated electric field intensity patterns at 784 nm of Au/Si nano-antenna structure. (a) Top view of the field patterns. (b) Lateral view of the field patterns.

In order to have an in-depth understanding of the physical image underlying the giant enhancement of absorption efficiency of Si, we calculate the field intensity distribution of the designed Au nano-antenna structure embedded with an Si nanoparticle at 784 nm. The results are plotted in Fig. 7. No matter from the top view or lateral view of the field patterns, we can find that the local field intensity is enhanced greatly and the strongest value always appears in the slot, with a maximum quantity of almost 13400, because of the local field enhancement features of surface plasmon resonance. As a result, there is a strong interaction between the Si particle and the incident optical field, which greatly increases the absorption cross section of Si accordingly.

3. Conclusions

In summary, our theoretical and numerical studies have shown that by taking advantage of the strong scattering and local field enhancement features of surface plasmon resonance, Au nanoparticles can effectively increase the absorption cross section of an Si nanoparticle in the near-infrared region. With the help of the designed 3D Au nanostructure, the absorption cross section of an Si particle can be enhanced by more than two orders of magnitude in the near-infrared band around 784 nm. In consideration of the role that Au nanoparticles play, we can regard them as a near-infrared light harvesting antenna. Our structure can be useful for applications in many areas such as optoelectronic detectors and optical sensing. The methodology can be applied to regulate and control the absorption band, such as increasing light absorption of mid-infrared and far-infrared region with other semiconductor materials and metals.

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