Enhanced light trapping in the silicon substrate with plasmonic Ag nanocones

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Ag nanocone enhanced light trapping in the silicon substrate is numerically investigated. For a wide range of the dielectric spacer thickness, the normalized scattering cross section of the rear located particles is higher than that of the front located particles, which is contrary to previous reports. This design not only avoids the conflict with the detrimental Fano effect but is also beneficial to the rear located particles. The fraction of the incident light scattered into silicon is calculated. The path length enhancement is assessed. The Ag nanocone shows highly competitive light-trapping potential. © 2013 Optical Society of America

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As a result of the localized surface plasmon resonance, metallic nanoparticle enhanced light trapping in silicon has been attracting tremendous attention because of important light-trapping applications, such as photovoltaic devices and solar energy [1–3]. By creating a collective oscillation of the conduction electrons in metal, the optical scattering cross section of metallic nanoparticles can be higher than their geometrical cross section at the resonance wavelength. The light trapping in silicon is enhanced. In previous reports, metallic particle shapes are commonly adopted as spheres, hemispheres, and cylinders. It is also usually seen that when the dielectric spacer is relatively thick (a too-thin dielectric spacer cannot often meet the requirements of devices [4]), the normalized scattering cross section $Q_{\text{scat}}$ (the scattering cross section is normalized to the geometrical cross section) for the front located particles is obviously higher than that for the rear located particles [5,6]. This suggests that it is beneficial to use the front located particles due to higher $Q_{\text{scat}}$. Unfortunately, the front located particles encounter a detrimental Fano effect, which reduces light absorption below the plasmon resonance wavelength because of the interference effects between the scattered light and the incident light [4,7–9]. Thus, higher $Q_{\text{scat}}$ with the front located particles is in conflict with the detrimental Fano effect. The rear located particles can avoid the Fano effect due to the strong absorption below the resonance [3,4]. But, the $Q_{\text{scat}}$ value of the rear located particles is lower than that of the front located particles, which is undesirable. Therefore, the ideal design is to make the $Q_{\text{scat}}$ value of the rear located particles higher than that of the front located particles for a wide range of the dielectric spacer thickness.

The light-trapping capability is critical for the applications of the light-trapping devices. The fraction of the incident light scattered into silicon is calculated by the power scattered into silicon divided by the total scatter power. The enhanced light-trapping potential can be assessed by calculating the optical path length enhancement compared to the path length for a single pass across the device [10]. In this Letter, the Ag nanocone is simulated to enhance light trapping in a silicon substrate.

An Al$_2$O$_3$ dielectric spacer is adopted due to its ideal passivation function, which produces the best result for high-efficiency, $n$-type crystalline silicon solar cells [11,12]. It is found that when the spacer thickness is 30 nm, the ratio of the $Q_{\text{scat}}$ value of the rear located particles to the front located particles has been near 2. This ratio is increased to 3 when the spacer thickness is reduced to 10 nm. In the meanwhile, Ag nanocones also show highly competitive light-trapping potential. Modern fabrication techniques have made the production of Ag nanocones possible [13].

Full-field electromagnetic simulations are performed with the finite-difference time-domain (FDTD) method by using the Numerical software package [14]. Figure 1 shows a single Ag nanocone placed on the top surface of an Al$_2$O$_3$ dielectric spacer with different thicknesses, which is on a semi-infinite crystalline silicon substrate. Perfectly matched layer (PML) boundary conditions are used on all axes. A total field scattered field source is employed. The scattering and absorption monitors are used to calculate the scattering cross section and the radiative efficiency. When light is incident on the particles from air, it corresponds to the front illumination and the particles are described as the front located particles. Likewise, when light is incident on the particles from the silicon substrate, it is described as the rear located particles.
located particles. For the rear located particles, the light source is positioned at a depth of 50 nm in silicon to minimize the amount of light absorbed in the silicon before arriving at the Ag nanocone. In the present model, both the bottom surface radius and the height of the nanocone are fixed at 50 nm for the sake of comparison with previous reports. The optical properties of Ag, crystalline silicon, and Al$_2$O$_3$ are obtained from Palik’s handbook [15].

$Q_{\text{scat}}$ is calculated for the front and rear located particles with Al$_2$O$_3$ spacer thicknesses of 30 and 10 nm as shown in Fig. 2. It is found that the $Q_{\text{scat}}$ value of the rear located particles is higher than that of the front located particles. When the Al$_2$O$_3$ spacer thickness is 30 nm, the ratio of $Q_{\text{scat}}$ between the rear to front located particles at the resonance wavelength has been near 2. This ratio increases to 3 when the Al$_2$O$_3$ spacer thickness is reduced to 10 nm. As the spacer thickness approaches zero from 10 nm, the ratio becomes higher. This difference in $Q_{\text{scat}}$ between the front and rear located particles is closely related with the high asymmetry in the conical shape along the incident light direction. The radiative efficiency, defined as the ratio of $Q_{\text{scat}}$ to $Q_{\text{ext}}$ (the normalized extinction cross section) at the resonance wavelength, is also calculated. When the thickness of the Al$_2$O$_3$ spacer is 30 nm, the radiative efficiencies are 51.6% and 55.0% for the front and rear located particles, respectively. When this spacer thickness is reduced to 10 nm, the efficiencies are increased to 60.4% and 61.8% for the front and rear located particles, respectively. This result indicates that the radiative efficiency for the front located particles is similar to that of the rear located particles but the scattering amount is the highest for the rear located particles.

Compared with the previous reports, it is often found that when the dielectric spacer is relatively thick, the $Q_{\text{scat}}$ value of the front located particles is higher than that of the rear located particles. For example, when the dielectric spacer thickness is in the range of 10–30 nm, $Q_{\text{scat}}$ of the front located particles is larger than that of the rear located particles, where the cylindrical particle shape and the SiO$_2$ dielectric spacer are used [6]. In this case, there exists a conflict of high $Q_{\text{scat}}$ at the front located particles with the detrimental Fano effect. Only when the dielectric spacer is reduced to an ultrathin thickness around 5 nm is the $Q_{\text{scat}}$ ratio between the rear to front located particles close to 2 [6]. But, in this case, such ultrathin dielectric spacers often are not able to meet the requirements of the light-trapping devices [4]. In contrast, the present design can make the $Q_{\text{scat}}$ value of the rear located particles significantly larger than that of the front located particles within a wider spacer thickness range from 0 to 30 nm.

The fraction of incident light scattered into the silicon substrate $F_{\text{abs}}$ is calculated. For comparison, the spherical and hemispherical Ag particles of 50 nm radius and the cylindrical Ag particles of a radius and a height of 50 nm are adopted from [10]. The calculation shows that $F_{\text{abs}}$ of the Ag nanocone is higher than that of the compared particle geometries for both the front and rear located particles. For comparison, the calculated $F_{\text{abs}}$ value of the front located particles is shown in Fig. 2, where the Al$_2$O$_3$ spacer thickness is 30 nm. It is seen that in the wavelength region of 600–1200 nm, $F_{\text{abs}}$ of the Ag hemispherical particles is slightly higher than that of the cylindrical particles. In addition, both are much higher than $F_{\text{abs}}$ of the Ag spherical particles. The trend is consistent with the report in the wavelength of 600–800 nm, where a 10 nm thickness SiO$_2$ spacer is used and $F_{\text{abs}}$ of the front located particles is reported [10]. This consistency shows that the replacement of the spacer materials does not affect the qualitative trend of $F_{\text{abs}}$ for these nanoparticle shapes.

The path length enhancement ($L$) is calculated by using the equation $L = 2d/(1 - F_{\text{abs}})$, where $d$ is a ratio of the average path length across a single pass of the device to the device thickness. Here, $F_{\text{abs}}$ is obtained from Fig. 3 and $d$ is obtained by performing a weighted integral of $1/\cos(\theta)$ over the angular distribution of the scattered power, where the $\theta$ is the angle along the normal direction of the coordinate system. It is found that when the thickness of the Al$_2$O$_3$ layer is 30 nm, the $L$ value of the nanocone is 22 for the front located particles at the wavelength of 800 nm whereas the hemisphere has an $L$ value of 18. When the Al$_2$O$_3$ layer thickness is reduced to 10 nm, the $L$ value for the nanocone is approximately 60, while the hemisphere is 35.

A quite-high fraction of the incident light is scattered into the silicon substrate rather than air. The far-field projection in the Cartesian coordinate system is calculated for the rear located nanocone with a 30 nm thick Al$_2$O$_3$ spacer at the wavelength of 1200 nm. Figures 4(a) and 4(b) show the far-field projection in the Cartesian and spherical coordinate systems, respectively. The far-field projection in the spherical coordinate system is calculated using the Mie scattering theory. The forward scattered intensity is obtained by setting the incident direction as the origin of the coordinate system. The spherical projection of the far-field intensity is calculated using the spherical Hankel function [15].
and 4(b) are the far-field projection in the silicon substrate and air, respectively. It is shown that the far-field distribution in the silicon substrate is fundamentally different from that in air. Furthermore, the highest field intensity in the silicon substrate is an order of magnitude higher than that in air. This is attributed to the asymmetrical dielectric environment surrounding the Ag nanocone.

In summary, the present design uniquely makes the $Q_{\text{scat}}$ value of the rear located particles remarkably higher than that of the front located particles in a wide range of the dielectric spacer thickness from 0 to 30 nm. It not only avoids the conflict of higher $Q_{\text{scat}}$ at the front located particles with the detrimental Fano effect but also provides higher light trapping in the silicon substrate. Modern fabrication techniques have made the construction of Ag nanocones possible. New light-trapping opportunities are offered from this design.

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