Enhanced optical absorption by Ag nanoparticles in a thin film Si solar cell*

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Thin film solar cells have the potential to significantly reduce the cost of photovoltaics. Light trapping is crucial to such a thin film silicon solar cell because of a low absorption coefficient due to its indirect band gap. In this paper, we investigate the suitability of surface plasmon resonance Ag nanoparticles for enhancing optical absorption in the thin film solar cell. For evaluating the transmittance capability of Ag nanoparticles and the conventional antireflection film, an enhanced transmittance factor is introduced. We find that under the solar spectrum AM1.5, the transmittance of Ag nanoparticles with radius over 160 nm is equivalent to that of conventional textured antireflection film, and its effect is better than that of the planar antireflection film. The influence of the surrounding medium is also discussed.

Keywords: transmittance, surface plasmon resonance, Ag nanoparticles, thin film solar cells

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1. Introduction

A key challenge for silicon-based solar cells is the weak absorption of long-wavelength photons near the bandgap (1.1 eV) due to the indirect bandgap of silicon.[1] A large fraction of the AM1.5 solar spectrum falls into a region (0.7 μm–1.1 μm) where silicon does not absorb light well. The trap of the long-wavelength photons brings a particular problem to the thin-film silicon solar cells. However, conventional texturing approaches have some limitations for their application to this field since the thickness of the absorbing layer restricts the depth of the surface texturing, which also increases the surface combination of carriers by increasing the surface area, thus degrading its functionality.[2] Therefore, a variety of approaches to increasing the optical absorptions in silicon-based solar cells have been investigated, with preference to light absorption and trapping mechanisms that do not increase the recombination losses. In this framework, the exploitation of the localized absorption of metal nanoparticles via surface plasmon resonance (SPR)[3–7] has been proposed for various solar cell configurations and photodetectors. Generally, the metal nanoparticles can be prepared by thermal evaporation,[8,9] electron beam evaporation,[10] sputtering[11] sol–gel method,[12] and so on.

In this paper we report on the exploitation of SPR metal nanoparticles coupled directly to silicon thin film solar cells. The influences of the Ag particle radius and the surrounding medium are also discussed. In our simulation, Ag nanoparticles are chosen because the plasma frequency of Ag is the lowest among noble metals, which is ideal for solar photovoltaic application.

2. Theory background

Generally, the Mie scattering theory can be used to simulate the scattering process of the nanoparticles. If any nanoparticles can be regarded as an ideal sphere and the interaction between the nanoparticles can be ignored, then the scattering coefficient $Q_{\rm sca}$, the extinction coefficient $Q_{\rm ext}$, and the absorption coefficient $Q_{\rm abs}$ can be expressed as follows:[13]

$$Q_{\rm sca} = \frac{\sigma_{\rm sca}}{\pi R^2} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)(|a_n|^2+|b_n|^2), \tag{1}$$

$$Q_{\rm ext} = \frac{\sigma_{\rm ext}}{\pi R^2} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)\,{\rm Re}(a_n+b_n), \tag{2}$$

$$Q_{\rm abs} = Q_{\rm ext} - Q_{\rm sca}, \tag{3}$$

where $x = 2\pi R/\lambda$, R the radius of the sphere, λ the incident wavelength; $\sigma_{\rm sca}$, $\sigma_{\rm ext}$, and $\sigma_{\rm abs}$ represent scattering cross section, extinction cross section, and absorption cross section, respectively; a_n and b_n are Mie coefficients and expressed as

$$a_n = \frac{m^2{\rm j}_n(mx)[x{\rm j}_n(x)]' - \mu_1{\rm j}_n(x)[mx{\rm j}_n(mx)]'}{m^2{\rm j}_n(mx)[x{\rm h}_n^{(1)}(x)]' - \mu_1{\rm h}_n^{(1)}(x)[mx{\rm j}_n(mx)]'}, \tag{4}$$

$$b_n = \frac{\mu_1{\rm j}_n(mx)[x{\rm j}_n(x)]' - {\rm j}_n(x)[mx{\rm j}_n(mx)]'}{\mu_1{\rm j}_n(mx)[x{\rm h}_n^{(1)}(x)]' - {\rm h}_n^{(1)}(x)[mx{\rm j}_n(mx)]'}. \tag{5}$$

Here, m is the refractive index of the sphere relative to the ambient medium; μ_1 is the ratio of the magnetic permeability of the sphere to the magnetic permeability of the ambient medium: often $\mu_1 = 1$; functions ${\rm j}_n(z)$ and ${\rm h}_n^{(1)}(z) = {\rm j}_n(z) + {\rm i}y_n(z)$ are spherical Bessel functions of order n ($n = 1, 2\ldots$) and of the given arguments, $z = x$ or mx, respectively; prime means derivative with respect to the corresponding argument.

From the above expressions, we conclude that in addition to the size factor, the SPR behavior of the nanoparticle also

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depends on the dielectric property of the sphere. According to Ref. [14], when the radius of the Ag sphere is larger than 10 nm, the dielectric property can be thought as the same as that of bulk and has no relationship with the size. So Ag data in Ref. [15] are used in simulation.

3. Discussion and results

3.1. Optimal distribution of Ag nanoparticles on a surface

Figure 1 shows the scattering spectra of different radii of Ag particles in the air. It can be seen from Fig. 1 that when the radius of the Ag sphere is 50 nm, the scattering spectrum only contains an electric dipole resonance peak, while as radius increases, the higher resonance mode begins to appear. For example, when the radius of Ag sphere is 80 nm, an electric quadrupole resonance peak appears; when the radius R exceeds 160 nm, an octupole resonance peak appears. Each of the scattering curves contains a minimum in 320-nm wavelength, which is due to the interband absorption in Ag. In view of scattering properties, the dipole scattering is isotropic; while for the higher mode, forward scattering is preferred to backward scattering. So the appearance of a higher mode resonance peak is more advantageous to enhance the absorption in the substrate. It can be supposed that nearly all scattering light can transmit when the radius of the particle is over 80 nm.

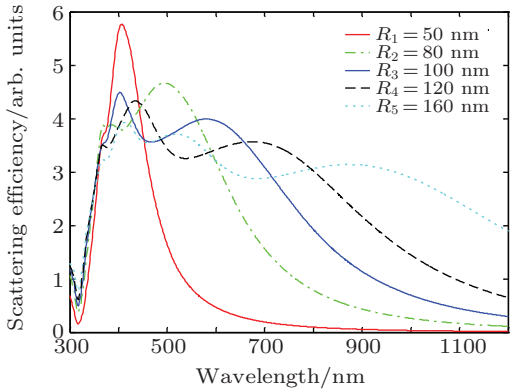


Fig. 1. (color online) Scattering efficiency curves for different radii of Ag nanoparticles in the air.

In practice, often the Ag nanoparticles are deposited on the surface of a thin film solar cell as shown in Fig. 2. If the radius of the Ag sphere is R, then the corresponding extinction cross section for a single sphere is $\pi R^2 Q_{\text{ext}}$. The substrate area is S. We suppose that the density of nanoparticles on the surface is σ. Under the uniform distribution condition, only when the extinction cross section of the metal nanoparticles is equal to the substrate area S, will the number of nanoparticles be optimal. Then we have

$$\sigma \cdot S \cdot \pi R^2 Q_{\text{ext}} = S, \tag{6}$$

and

$$\sigma(\lambda) = \frac{1}{\pi R^2 Q_{\text{ext}}(\lambda)}. \tag{7}$$

By using the above equation, we can calculate the density distribution corresponding to a particular radius R and a specific wavelength. If the density σ increases further, the adjacent particles are so close to each other that the light illumination on each particle cannot be fully utilized to excite the surface plasmons. According to Eq. (7), the optimal transmittance T is

$$T = \frac{\sigma \cdot S \cdot \pi R^2 Q_{\text{sca}}}{S} = \frac{Q_{\text{sca}}}{Q_{\text{ext}}}. \tag{8}$$

Obviously the transmittance T is a function of wavelength, and it is also dependent on the density distribution. In the latter calculation, we assume that the density distribution of the Ag nanoparticles is optimal, so T is determined only by the scattering-to-extinction ratio.

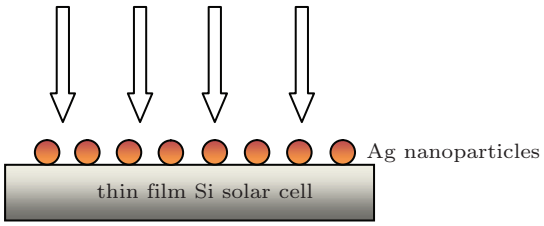


Fig. 2. (color online) Ag nanoparticles on the substrate.

3.2. Influence of the Ag nanoparticles with different radii

In Fig. 3, the curve of the optimal transmittance versus wavelength for $R = 100$ nm, and transmittance curves for other different antireflection coatings are listed. As contrast, the ZnO film is selected because this layer is one of the most popular films used in thin film solar cells and SiN_x film is popularly used in crystalline silicon solar cells. The data of ZnO and SiN_x films are cited from documents in AFors-Het software. In Fig. 3, we can find that compared with using the conventional antireflection coating, the use of Ag nanoparticles can effectively enhance the transmittance in the long wavelength

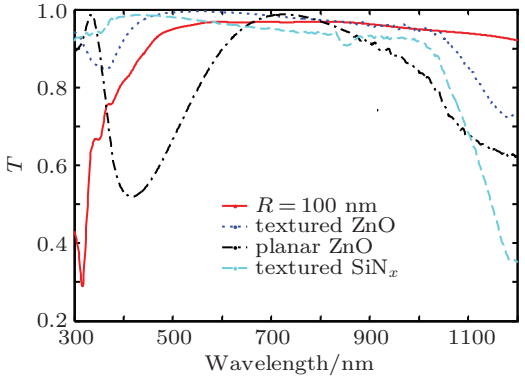


Fig. 3. (color online) Comparisons of transmittance curves for different layers, where the solid line, the dotted line, the dashed line, and the dashed–dotted line represent transmittance curves for Ag nanoparticles with $R =$ 100 nm, the textured ZnO, the textured SiN_x, and the planar ZnO, respectively.

band, especially in a region of 1000 nm–1200 nm, while because of the absorption by Ag atoms at 320 nm, the transmittance near 320 nm is much lower than those of conventional antireflection films.

In order to compare the transmittance capability of Ag nanoparticles with that of conventional antireflection coating, combining the light intensity distribution in the solar spectrum AM 1.5, an enhanced transmittance factor $\bar{T}$ is introduced as follows:[16]

$$\bar{T} = \frac{\int_{300}^{1200} (T - T_0) S(\lambda) \mathrm{d}\lambda}{\int_{300}^{1200} S(\lambda) \mathrm{d}\lambda}, \tag{9}$$

where T_0 represents the transmittance of conventional antireflection coating, and $S(\lambda)$ is the intensity distribution.

Table 1 shows the transmittance comparison between the Ag nanoparticles and antireflection coatings. Combining Fig. 1 and Table 1, we can find that with the radius of nanoparticle increasing, the scattering spectrum of the metal nanoparticles extends toward longer wavelength. So when the particle radius is over 80 nm, the transmittance first improves markedly; however, with the further increase of particle radius, the transmittance effect becomes saturated. If the radius of Ag is 180 nm, the transmittance effect of Ag nanoparticles is 13.08% higher than that of the planar ZnO layer, and is 3.16% better than that of the textured SiN_x layer, but is 0.37% lower than that of the textured ZnO film. These results suggest that the transmittance of the metal nanoparticles is much better than that of the planar antireflection film, and its influence is nearly the same as that of textured antireflection coating.

Table 1. The comparisons of enhanced transmittance factor between Ag nanoparticles with different radii and the conventional antireflection coating.

Sphere radius/nm	$\bar{T}$ for textured ZnO/%	$\bar{T}$ for textured-SiN_x/%	$\bar{T}$ for planar ZnO/%
80	–3.94	–0.40	9.51
100	–1.92	1.62	11.53
120	–1.09	2.45	12.36
160	–0.50	3.03	12.94
180	–0.37	3.16	13.08

3.3. Influence of the dielectric surrounding

Because of unique optical and electrical properties of SPR, this technique is widely used in thin film solar cells, but there are still many problems to be solved, such as the pollution problems caused by metal nanoparticles. Ag spreads very rapidly in silicon and it is easy to become an effective recombination center, so usually the Ag particles need to be surrounded by an insulating medium to avoid the direct contact with Si. At this time, the ambient medium changes from air into the insulating medium. In Fig. 4, the solid line represents the transmittance curve for Ag particles with $R = 100$ nm surrounded by SiN_x. We can find that when the surrounding medium is SiN_x, the transmittance over the entire spectrum decreases distinctly, especially in short band $\lambda < 600$ nm. These can be deduced from Eq. (4), when the refractive index of the medium around the metal nanoparticles increases, m will drop, which results in the decrease of the scattering coefficient and the transmittance. The variation of transmittance with the nanoparticle size is listed in Table 2.

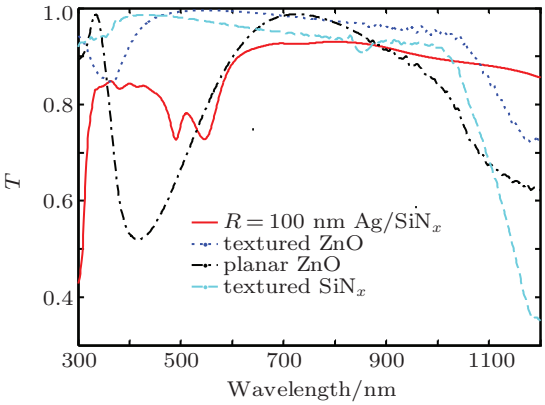


Fig. 4. (color online) Comparisons of transmittance curves for different layers, where the solid line, the dotted line, the dashed line, and the dashed–dotted line represent transmittance curves for Ag nanoparticles with $R = 100$ nm in SiN_x, the textured ZnO, the textured SiN_x, and the planar ZnO, respectively.

Table 2. Comparisons of enhanced transmittance factor between Ag nanoparticles with the surrounding medium SiN_x and the conventional antireflection coating.

Sphere radius/nm	$\bar{T}$ for textured ZnO/%	$\bar{T}$ for textured-SiN_x/%	$\bar{T}$ for planar ZnO/%
100	–9.40	–5.86	4.04
120	–7.17	–3.63	6.27
140	–6.00	–2.47	7.44
160	–5.27	–1.73	8.18
180	–4.73	–1.19	8.72

When the environmental medium is replaced by SiO_2, the detailed data are shown in Table 3.

Table 3. Comparisons of enhanced transmittance factor between Ag nanoparticles with the surrounding medium SiO_2 and the conventional antireflection coating.

Sphere radius/nm	$\bar{T}$ for textured ZnO/%	$\bar{T}$ for textured-SiN_x/%	$\bar{T}$ for planar ZnO/%
100	–4.82	-1.28	8.62
120	–3.49	0.04	9.95
140	–2.86	0.67	10.58
160	–2.50	1.03	10.94
180	–2.25	1.28	11.19

Comparing the results listed in Table 2 and Table 3, we find that with the decrease of the refractive index of surrounding medium, the increase of m corresponds to the increase of the transmittance. When the surrounding medium is SiO_2, if the radius of Ag is 180 nm, the transmittance of Ag nanoparticles is 1.28% higher than that of textured SiN_x and is 2.25%

lower than that of textured ZnO. The computation results show that when the Ag nanoparticles are surrounded by insulating medium, the higher the refractive index of the medium, the lower the transmittance is. So if it is necessary to use the surrounding medium, the material with lower refractive index is preferred.

4. Conclusions

In this paper, the Mie theory is used to simulate the scattering properties of Ag nanoparticles. When the metal nanoparticles are used in the surface of a thin film solar cell, with the radius increasing from 80 nm to 160 nm, the transmittance increases markedly; while with radius further increasing, the transmittance is nearly saturated. Comparing the transmittance capability of Ag nanoparticles with that of conventional antireflection coatings, we find that the transmittance of Ag nanoparticles is nearly the same as that of textured antireflection film, and its effect is much better than that of planar antireflection film. If the metal nanoparticles need to be surrounded by an insulating medium, the medium with lower refractive index is preferred.

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