

Hetero-structured lumpy nanoparticle conformal structure for high absorbance of ultrathin film amorphous silicon solar cells

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We present a concept for enhancing the absorbance of amorphous-silicon solar cells by using hetero-structured nanoparticles consisting of dielectric core particles combined with small metallic surface nanoparticles half embedded in the core to harness both the scattering effect and the near field light concentration. Through optimising key parameters, including the relative distance of the nanoparticles to the solar cell, the radius ratio of the core to the surface nanoparticles, and the refractive index of the core particles, the short circuit current density in a 20 nm nanoparticle-integrated active layer is equivalent to that in a 300 nm flat active layer. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4851238>]

The recent progress in nano-plasmonics has offered a great potential for advancing the photovoltaics and, in particular the thin film technology, for much improved device performance.^{1–4} Metallic nanostructures or nanoparticles have been integrated into the solar cell architecture to effectively enhance the light absorption in the active layer by either the resonant scattering or the near-field concentration.^{5–7} Significant boosts in the photocurrent, the fill factor, and the open circuit voltage have been achieved.⁸ However, the following key challenges of using the plasmonic effect in solar cells have remained unsolved. First, the resonant scattering is always accompanied with the intrinsic absorption loss from the metal nanostructures/particles offsetting the benefit from plasmonic enhancement. Second, simultaneously harnessing the scattering and near field enhancements is difficult because the required particle size and geometry are largely different for these two effects.²

Recently, the nucleated nanoparticle geometry (or the lumpy geometry) was demonstrated to be an effective way to mitigate these challenges in thin film solar cells.^{9–11} Through combining a large core Ag particle with a number of small Ag surface nanoparticles, the strong scattering effect and the near field effect can be enabled leading to a significant enhancement of more than 20% in the solar cell conversion efficiency. However, the intrinsic absorption and the light blockage from the silver nanoparticles cannot be avoided, limiting the integration of the nucleated nanoparticles only to the back contact layer of the thin film solar cells.

In this paper, we propose a hetero-structured lumpy nanoparticle model, as shown in Fig. 1, to address the challenges associated with the plasmonic nanoparticles in amorphous silicon (a-Si) thin film solar cells. For the core particles, metallic materials are replaced by dielectric materials to achieve strong broadband scattering with negligible particle absorption. Nanometer sized metal nanoparticles are used as the surface particles to enable the near field concentration.^{12,13} In the hetero-structured lumpy nanoparticles, 26

small metallic spheres are evenly anchored half embedded surrounding the outside of the large dielectric core particles. Due to the minimized nanoparticle absorption and the light blockage, these hetero-structured lumpy nanoparticles can be closely packed between the front surface of a-Si layer and the indium tin oxide (ITO) layer to enhance the absorption in the solar cell. The benefit of the closely packed hetero-structured lumpy nanoparticles on the front surface of solar cells also lies in the effective anti-reflection effect in the far field to further improve the light trapping.^{14,15} It has been found that the relative distance of the center of the hetero-structured nanoparticles to the top surface of the a-Si layer and the size of the core dielectric particles play a crucial role on the light absorption enhancement. The maximum absorbance gain of 50.7% relative to the unmodified a-Si layer is achieved with the optimized position and size of the hetero-structured nanoparticles. To further enhance the near-field effect, an ultrathin conformal solar cell geometry based on the hetero-structured nanoparticles is proposed. In this case, a 20 nm thick a-Si active layer can absorb nearly the same solar energy as that for a 300 nm thick a-Si active layer in a standard solar cell with an anti-reflection coating. The findings in this paper have the great potential to dramatically reduce the cost of the silicon thin film solar cell at a remained high efficiency.

Fig. 1 shows the schemes of the model for a-Si thin film solar cell with closely packed hetero-structured lumpy nanoparticles sandwiched between the a-Si layer and the ITO layer. The model was simulated with the Lumerical FDTD software, and the dielectric functions were from the Palik handbook.¹⁶ The solar cell was set up according to the common silicon thin film solar cell geometry (ITO: 20 nm, a-Si: 300 nm, ZnO:Al: 100 nm, and Ag: 180 nm).¹⁷ The hetero-structured nanoparticle was designed with a large dielectric core particle covered by nanometric metallic nanoparticles half embedded in the dielectric core. A broadband plane wave source (300 nm–800 nm) was used to simulate the light incident on the particles from the top. The relative distance d and the radius ratio α (the ratio of the radius of the dielectric core to that of the metallic particles) were investigated in the

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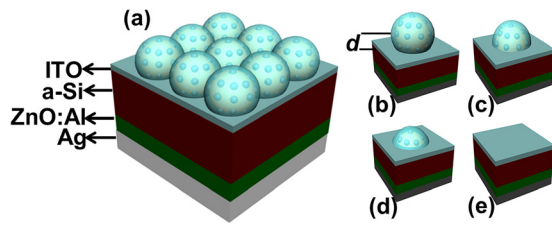


FIG. 1. (a) The scheme of the simulation model. (b)–(e) The solar cell structures with the hetero-structured nanoparticles sandwiched between the top surface of the a-Si layer and the ITO layer with different relative distances.

simulation. d was changed from $-R$ to R (R is the effective radius of the hetero-structured nanoparticle), as shown in Figs. 1(b)–1(e). The radius ratio α was changed from 50/10 to 200/10. Periodic boundary conditions (PBCs) were used at the lateral boundaries of the simulation model to mimic the infinite periodic arrays of nanoparticles.

SiO_2 was selected to demonstrate the primary concept of the hetero-structured nanoparticles because its refractive index ($\text{RI} \approx 1.5$) is between air and a-Si ($\text{RI} \approx 4$) and it is almost lossless in the visible spectrum. In addition, SiO_2 nanoparticles have been proven to be effective in light trapping and anti-reflection.^{18,19} As the near field light concentration of Ag nanoparticles in thin film solar cells^{6,7} can lead to the enhanced electric field and thus result in photogeneration excitation increase, we select Ag nanoparticles with 10 nm radius as the surface metallic particles.

To quantify the effect of the hetero-structured nanoparticles on the absorbance of a-Si solar cells, we first calculated the absorbance of the a-Si $A(\lambda)$, which is defined as the ratio of the power of the absorbed light $P_{abs}(\lambda)$ to that of the incident light $P_{in}(\lambda)$ within the a-Si film

$$A(\lambda) = P_{abs}(\lambda)/P_{in}(\lambda). \quad (1)$$

The power absorbed can be written as

$$P_{abs}(\lambda) = \frac{1}{2} \omega \varepsilon'' |E|^2. \quad (2)$$

Here, ω is the frequency, ε'' is the imaginary part of the permittivity, and E is the electric field. Then by integrating the absorbance with the AM 1.5 solar spectrum, we can get the area independent short circuit current density (J_{SC}), assuming that all generated electron-hole pairs contribute to the photocurrent

$$J_{SC} = e \int (\lambda/hc) A(\lambda) I_{AM1.5}(\lambda) d\lambda, \quad (3)$$

where e is the electron charge, h is Plank's constant, c is the speed of light in free space, and $I_{AM1.5}$ is AM 1.5 solar spectrum. The absorption enhancement G in the 300 nm thick a-Si film with/without the hetero-structured nanoparticles is calculated and compared by changing the relative distance and the radius ratio

$$G = A_{withNP}(\lambda)/A_{ref}(\lambda), \quad (4)$$

where $A_{withNP}(\lambda)$ represents the absorbance of the a-Si film with the hetero-structured nanoparticles, and $A_{ref}(\lambda)$

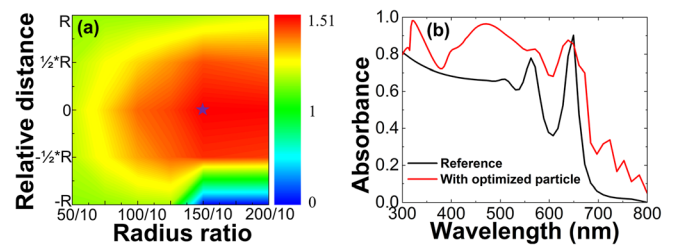


FIG. 2. (a) Absorption enhancement in the a-Si layer with/without the hetero-structured nanoparticles as a function of the relative distance d and the radius ratio α . (b) Light absorbance in the a-Si layer with/without the hetero-structured nanoparticles at the optimized position in (a).

represents the absorbance of the a-Si layer without the hetero-structured nanoparticles.

To find out the optimized hetero-structured nanoparticles and the best position of the particles to the solar cells for a maximum absorption enhancement in the a-Si layer, we systematically investigated two parameters: the radius ratio α and the relative distance d . Based on the scattering effect from dielectric nanoparticles^{20,21} and our previous results with Ag nanoparticles on the front surface of solar cells for enhanced near-field effect, the radius ratios are selected to be 50/10, 75/10, 100/10, 125/10, 150/10, 175/10, and 200/10. The relative distance is changed from R to $-R$, as shown in Figs. 1(b)–1(f). By mapping the absorbance as a function of the radius ratio and the relative distance, the optimized condition for the largest absorption enhancement in the a-Si layer is found as shown in Fig. 2(a). It can be seen that the highest absorption enhancement of $G = 1.507$ is located at the purple star point under the optimized parameters with $d = 0$ and $\alpha = 150/10$. It can also be seen that when the particles are partially embedded in the a-Si layer, the absorption enhancement is larger than the case when the particles are on the top of the a-Si surface or totally embedded in the a-Si layer. That is mainly because that the forward scattering from the hetero-structured nanoparticles is improved when they are partially embedded in the a-Si layer. In addition, they can act as a high performance anti-reflection coating due to the graded RI matching. The light absorbance as a function of the wavelength is calculated and shown in Fig. 2(b). It can be seen that compared with a reference a-Si layer without the hetero-structures nanoparticles the absorption enhancement is over the entire investigated wavelength range and the integrated absorbance can be enhanced as much as 50.7%.

The achieved large absorption enhancement allows us to further investigate the solar cells with a reduced active layer

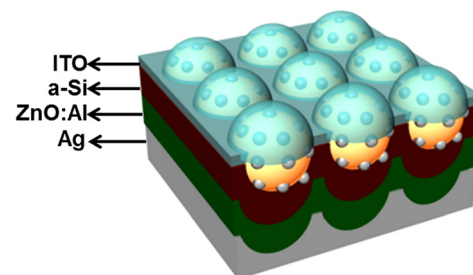


FIG. 3. The schematics of the conformal structure for the ultrathin a-Si solar cell.

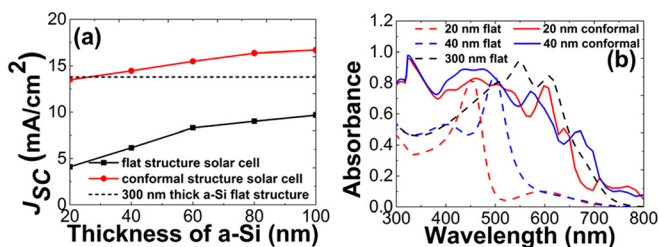


FIG. 4. (a) J_{SC} in the conformal solar cell structure as a function of the a-Si thickness. (b) Absorbance in the a-Si layers as a function of the wavelength for different thicknesses.

thickness. Based on the above optimization results, we propose a conformal structure^{22,23} to investigate the light absorbance in the ultrathin a-Si layer as shown in Fig. 3. The a-Si layer and the other layers in the solar cell follow the hemispherical shape of the hetero-structured particles half embedded in the a-Si layer. The J_{SC} in the conformal solar cells of the a-Si layer with different thicknesses (from 20 nm to 100 nm) is calculated and compared to the standard solar cells with a 80 nm ITO anti-reflection layer on the top, as shown in Fig. 4(a). It can be observed that the J_{SC} is tripled in the conformal structure compared with that of a standard solar cell configuration with the same active layer thickness due to the enhanced light trapping effect. At the point of the 20 nm thickness of the a-Si layer, the J_{SC} is increased from 4.11 mA/cm² to 13.5 mA/cm², which is comparable with the maximum achievable J_{SC} in the standard flat 300 nm thick a-Si solar cell (13.8 mA/cm²), as indicated by the dashed horizontal line in Fig. 4(a). The boost in J_{SC} is attributed to a combination of the scattering effect, the anti-reflective properties of the closely packed dielectric nanoparticles, which are half embedded in a-Si layer and also the enhanced electric field in the vicinity of the small Ag nanoparticles due to the near field light concentration.

Fig. 4(b) shows the absorbance of the 20 nm and 40 nm thick a-Si layers in the conformal solar cells as a function of the wavelength compared with a standard solar cell structure with the same thicknesses of the a-Si layer. In Fig. 4(b), the absorbance of a standard 300 nm thick a-Si solar cell is also presented for comparison. It can be seen from Fig. 4(b) that the absorption of the a-Si layer in the conformal structure is enhanced through the overall wavelength range compared with those in the standard cells due to the comprehensive role of the hetero-structured lumpy nanoparticles. The enhancement in the shorter wavelength range is the highest because of the low absorption loss from the SiO₂. The absorbance of a 20 nm

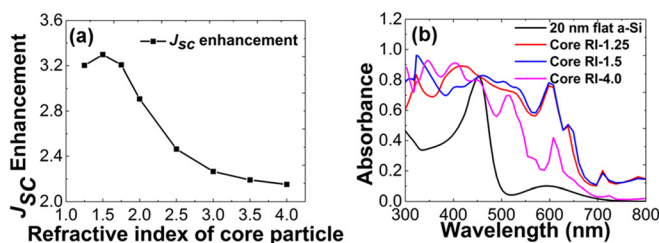


FIG. 6. (a) Normalized J_{SC} enhancement in the conformal structure solar cell with 20 nm thick a-Si layer as a function of the RI of the core particles. (b) Absorbance in the 20 nm thick a-Si layer in the conformal structure for core particles with different RIs as a function of the wavelength.

thick a-Si conformal solar cell is comparable with that for a standard 300 nm thick flat a-Si solar cell. Thus, it can be concluded that the conformal structure with the hetero-structured nanoparticles can offer a much effective light trapping strategy than the traditional anti-reflection coating of a-Si solar cell.

To further confirm the mechanism for the enhanced absorption, the electromagnetic field intensity distributions in the 20 nm conformal a-Si layer with and without the small Ag nanoparticles are calculated and shown in Fig. 5. The polarization of the incident light is in the X direction and the field component of light is also along the X direction. It can be clearly seen in Fig. 5 that no obvious absorption loss is observed in the SiO₂ particles due to the lossless nature of the SiO₂¹⁶ in the interested wavelength range. The calculation results clearly show that two main physical mechanisms are responsible for the observed absorption enhancement in the a-Si layer. First of all, the conformal structure induced by the SiO₂ leads to strong near-field coupling to guided modes supported by the multi-layer solar cell structure.^{13,24} This can be observed even without the presence of the Ag nanoparticles in Figs. 5(a)–5(c). Second, the surface Ag nanoparticles introduce the strong local field concentration in the close vicinity of the nanoparticles leading to further absorption enhancement in the a-Si layer as compared to Figs. 5(a)–5(c), in particular at 500 and 600 nm, where the peak of the solar spectrum is located. Therefore, both the dielectric core particle and the surface Ag particles in the hetero-structured nanoparticles play an important role in achieving the significant absorption enhancement in the a-Si layer.

In the hetero-structured nanoparticle design, the dielectric core particles are important in determining the strength of the light scattering and anti-reflection. In addition to the size and geometry, the RI plays an important role in the light

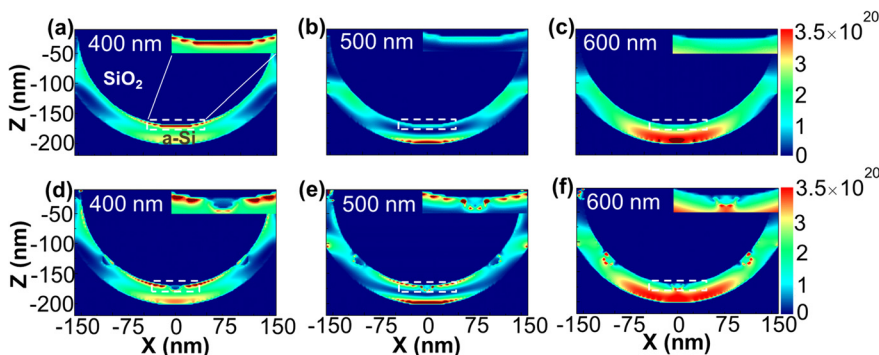


FIG. 5. Electric field intensity distributions of a-Si solar cells with (a)–(c) SiO₂ core only conformal geometry and (d)–(f) hetero-structured lumpy nanoparticle conformal geometry. Insets: highlight of the close vicinity of the Ag nanoparticles.

trapping. To further optimize the design of the hetero-structured nanoparticles on the absorbance of a-Si in conformal structure, the RI of the core particles is investigated from 1.25 to 4.0 and the thickness of the a-Si layer is set at 20 nm. Fig. 6(a) shows the J_{SC} enhancement as a function of the RI of the core particles. The optimized RI of the core particles to achieve the best enhancement of J_{SC} is 1.5 with a relative absorption enhancement of 229.8% compared with that in the flat 20 nm thick a-Si solar cell case. By further increasing the RI of the core particles, the J_{SC} enhancement decreases due to the reduced anti-reflection and scattering effect. Fig. 6(b) shows absorbance as a function of the wavelength with the RI of the core particles at 1.25, 1.5, and 4.0, respectively. From Fig. 6(b), we can see that the absorption in ultrathin a-Si layer with the core particles of a higher RI decreases at the wavelength above 450 nm, leading to a reduction in the absorption enhancement.

In summary, this paper introduces an approach for a broadband absorption enhancement in the a-Si thin film solar cells by placing the hetero-structured nanoparticles on the front side of solar cells. The proposed conformal structures enable significant J_{SC} gains of 229.8% in the 20 nm thick a-Si solar cell by simultaneously harnessing the strong scattering from large dielectric nanoparticles with a RI at 1.5 and near field light concentration from small Ag nanoparticles. The absorbance of an optimized 20 nm thick a-Si conformal solar cell with the hetero-structured nanoparticles can be comparable with a 300 nm thick standard a-Si solar cell with the conventional anti-reflection coating.

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