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Photocurrent improvement of an ultra-thin silicon solar cell using the localized surface plasmonic effect of clustering nanoparticles

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The cluster-shaped plasmonic nanostructures are used to manage the incident light inside an ultra-thin silicon solar cell. Here we simulate spherical, conical, pyramidal, and cylindrical nanoparticles in a form of a cluster at the rear side of a thin silicon cell, using the finite difference time domain (FDTD) method. By calculating the optical absorption and hence the photocurrent, it is shown that the clustering of nanoparticles significantly improves them. The photocurrent enhancement is the result of the plasmonic effects of clustering the nanoparticles. For comparison, first a cell with a single nanoparticle at the rear side is evaluated. Then four smaller nanoparticles are put around it to make a cluster. The photocurrents of 20.478 mA/cm^2, 23.186 mA/cm^2, 21.427 mA/cm^2, and 21.243 mA/cm^2 are obtained for the cells using clustering conical, spherical, pyramidal, cylindrical NPs at the backside, respectively. These values are 13.987 mA/cm^2, 16.901 mA/cm^2, 16.507 mA/cm^2, 17.926 mA/cm^2 for the cell with one conical, spherical, pyramidal, cylindrical NPs at the backside, respectively. Therefore, clustering can significantly improve the photocurrents. Finally, the distribution of the electric field and the generation rate for the proposed structures are calculated.

Keywords: clustering nanoparticles, plasmonic solar cell, localized surface plasmon resonance, photocurrent, finite difference time domain (FDTD) method, light management

PACS: 84.60.Jt, 82.35.Np, 88.40.H– **DOI:** 10.1088/1674-1056/ab836d

1. Introduction

There are outstanding advantages for renewable energy sources because they are widely available and inexpensive over the planet. Solar energy plays an essential role in a wide range of renewable energy sources, and many investments have been made in research to improve efficiency of solar cells.[1–12] However, price of electricity from solar energy is higher than the energy produced by conventional energy sources.[13–15] By combining low production costs and reasonable performance, thin-film photovoltaics are an attractive option to reduce the total cost per Watt of solar energy.[14,16] Silicon is the main material for photovoltaic applications because of its low cost, abundance in nature, non-toxicity, long-term stability, and well-established technology.[17,18] However, to build large photovoltaic modules, its cost should be significantly reduced. Light trapping can be used to reduce the physical thickness of photovoltaic active layers.[19–22] One of the important ways of light trapping is using plasmonic structures.[23–25] Recently, there appear a greatly increasing number of studies on the plasmonic nanostructures[26–30] because of their good prospects for applications in such systems to solve several practical nano-electronics problems. Local fields arising near such structures as a result of plasma oscillations of the conduction electrons of noble metals arouse the interest of researchers to use them in optoelectronic devices.[31–34] In the case of solar cells, plasmonic nanoparticles have been used to design ultra-thin film solar cells.[35–37] In several works, plasmonic nanoparticles have been placed on the surface, inside or backside of the active layer, to improve the cell performance.[20,38–40] Noble metals such as gold and silver, whose mobile electrons can move between the ion lattice, have been used in the field of photovoltaics.[41] By applying the electric field, the electrons diverge with negative loads in one direction, and at the same time, they return to the lattice ions with a tensile force.

In fact, in an appropriate phase change, an electron oscillation resonance occurs in response to the electric field. This electron oscillation resonance is the same as plasmon, which is used in the physics of plasmonic. It can be said that plasmons cause some nanoparticles to interact with light.[42] Management of optical losses in the ultra-thin-film solar cells by using plasmonic nanoparticles is an important issue. This helps us to design a cell with better absorption of the incident light. It is known that a silicon solar cell has a relatively weak absorption coefficient.[15] Thus, to design a thin-film silicon solar cell, a manipulation is needed. This problem can be solved using plasmonic nanoparticles. Further progress in this area is impossible without the development of a proper simulation of new kinds of nanoparticles and their applications in the field of photovoltaics. The idea of this paper is to utilize plasmonic nano-clusters. They can be made from coupled metallic nanoparticles. Clustering significantly enhances the absorption spectra, giving rise to highly localized near fields.[43–45] Nano-clustering has been used in some applications such as biosensors, optical four-wave mixing.[46,47] Today, the self-

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assembly fabrication processes are a way that enables us to fabricate clustering nanostructures. In Ref. [48] it was shown that the self-assembled clusters of spherical shape nanoparticles can be fabricated, for use in the nanophotonic structures. In the present work, we investigate the effect of cluster-shaped nanoparticles on the absorption spectra of an ultra-thin film silicon solar cell. The cylindrical, spherical, conical and pyramidal-shaped nano-clusters are used. Our goal is to improve the absorbed power. Finally, we try to show that the clustering method of plasmonics is capable of significantly improving solar cell efficiency.

2. The structure design and simulation methodology

Noble metal nanostructures can be produced in the desired composition, size, and shape, with different properties. In previously published works, it is demonstrated that using localized surface plasmons effect of an array of metallic nanoparticles can improve the performance of a thin-film solar cell. For instance, in Ref. [49] a single Ag nanoparticle on a substrate was simulated. Here, the main aim is to show the effect of the clustering effect on the performance of a thin-film solar cell. For more clarification, in Figs. 1(a) and 1(b), the difference between the array of nanoparticles and an array of clustering is depicted.

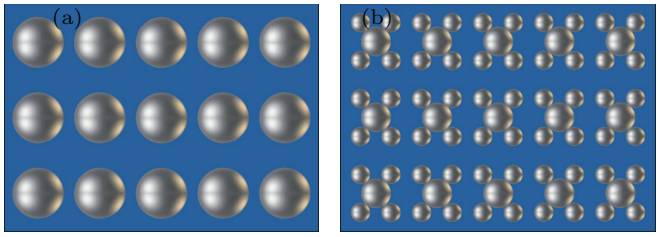


Fig. 1. (a) An array consisting of single nanoparticles, and (b) an array consisting of clustering nanoparticles.

It is important to mention that the volume of a single nanoparticle is $\frac{4}{3}\pi R_{\text{single}}^3$ in a unit cell and that is $\frac{4}{3}\pi(R^3+4r^3)$ for clustering nanoparticles where the radius of the central nanoparticle is R and the radii of surrounding nanoparticles are r. In the case of nanoparticles when R_{single} is higher than R, it may yield a bigger volume for a single nanoparticle in comparison to clustering nanoparticles. Therefore, it is possible to design a cell using clustering nanoparticles with a lower volume ratio. Use and design of cluster-shaped metal nanoparticles are the main aims of this work. Clustering is made using cylindrical, spherical, conical, and pyramidal nanoparticles in the rear side, as shown in Figs. 2(a)–2(d), respectively. Here one large nanoparticle is placed at the center of the nano-cluster with four smaller nanoparticles around it. We hope that assembling nanoparticles as a nano-cluster will result in more improvement, compared to the cases in which a single nanoparticle is used. The thickness of the active layer is 300 nm and 400 nm, and the period is 300 nm and 400 nm. Moreover, an ultra-thin SiO_2 layer with thickness 80 nm is used as a substrate layer. A cell with a volume of $400\times400\times400$ nm^3 is considered and the simulation is carried out for four cases. In case I, a sizeable pyramidal-shaped nanoparticle is placed at the center of a nano-cluster with four smaller ones around it (see Fig. 2(a)). In case II, a spherical-shaped nanoparticle with a radius of 100 nm is placed in the center of nano-cluster with four spherical-shaped nanoparticles in radii of 50 nm around it (see Fig. 2(b)). In case III, a conical-shaped nanoparticle with a radius of 100 nm and a height of 200 nm is placed in the center of nano-cluster surrounded by four conical-shaped nanoparticles with radii of 37.5 nm and height of 150 nm (see Fig. 2(c)). Finally, in case IV, a cylindrical-shaped nanoparticle with a radius of 130 nm and a height of 86 nm is located in the center of nano-cluster and is surrounded by four cylindrical-shaped NPs with radii of 70 nm and height of 35 nm (see Fig. 2(d)). Furthermore, the simulation is repeated for cell dimensions of $400\times400\times300$, $300\times300\times400$, and $300\times300\times300$ nm, respectively. For comparison, a cell without any nanoparticles is simulated as well.

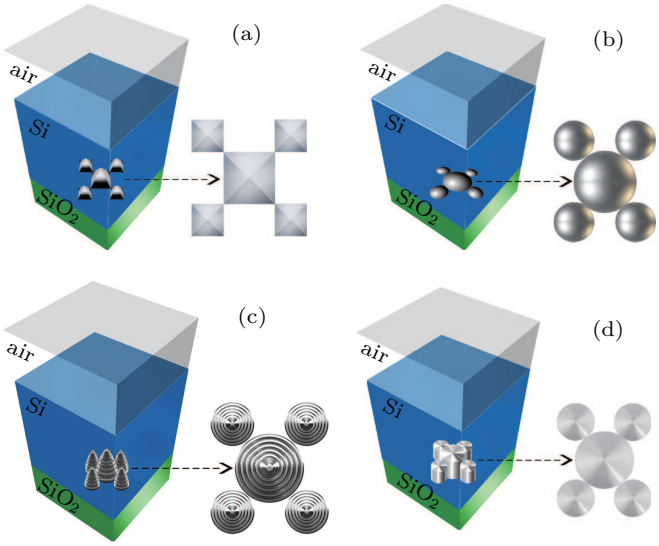


Fig. 2. Schematic diagrams of simulated plasmonic silicon solar cell with (a) clustering pyramidal-shaped Ag nanoparticles at the backside, (b) clustering spherical-shaped Ag nanoparticles at the backside, (c) clustering conical-shaped Ag nanoparticles at the backside, (d) clustering cylindrical-shaped Ag nanoparticles at the backside.

The absorbed power, short-circuit current density and electric field distribution are calculated using the finite-difference time-domain (FDTD) method.[50] A perfectly matched layer (PML) was used for upper and lower boundary conditions and periodic boundary conditions for lateral boundaries. A plane wave source was used in the wavelength range from 0.3 μm to 1.1 μm. The absorbed power is calculated by the absorption spectrum formula[38]

$$A(r,\lambda) = \frac{1}{2}\frac{\text{Re}(\nabla P)}{P_{\text{in}}} = \frac{1}{2}\frac{\omega\text{Im}(\varepsilon(r,\omega))\,|E(r,\omega)|^2}{P_{\text{in}}}, \quad (1)$$

where E is the electric field, P_{in} is the incident light power, ω is the angular frequency, and ε is the dielectric constant. To calculate the current, the optical production rate was calculated according to wavelength. The absorption spectrum $A(r,\lambda)$ was calculated with the formula $A(\lambda) = \int A(r,\lambda)\mathrm{d}V$. The short-circuit current is obtained by the following equation:

$$J_{\text{SC}} = q\int_{0.4}^{1.1} \frac{I(\lambda)}{\lambda} A(\lambda)\mathrm{d}\lambda, \tag{2}$$

where $I(\lambda)$ is the intensity of the incident light. Finally, the electric fields for the structures of metal nanoparticles were studied. This shows us how nanoparticles stimulate the electrons around themselves.

3. Results and discussion

Clustering nanoparticles are used to improve the photocurrent of an ultra-thin silicon solar cell. The interaction of the incident light as an electromagnetic field and clustering nano-particles is the main reason for improvement. Due to their shape, size, material, and other factors, the absorption enhancement can be obtained at different wavelengths. First, for comparison, a 400 nm silicon solar cell is simulated without any nanoparticles. Then, clustering the nanoparticles is used to design an ultra-thin solar cell with a photocurrent as high as possible. Figure 3(a) shows the top view of the pyramidal-shaped nano-cluster that is used in the backside of the active layer of the Si solar cell with thickness of 400 nm. Figure 3(b) compares its absorption spectrum with the reference cell as well as a cell with a pyramidal-shaped nanoparticle in its backside. As is seen, clustering nano-particles improves the absorption spectra more than a single nanoparticle.

Then clustering spherical-shaped nanoparticles are used to improve the performance of a cell with thickness of 400 nm in its backside. These clustering nanoparticles are shown in Fig. 4(a). The absorption spectra of this cell are depicted in Fig. 4(b), which are compared with the absorption spectra of a cell with one spherical nanoparticle as well as with the reference cell. As can be seen, cluster-shaped spherical NPs mainly improve the absorption spectrum at wavelengths higher than 500 nm. This is because high energy photons (low wavelengths) are absorbed near the front surface of the absorber and low energy photons (high wavelengths) are absorbed in the rear side of the absorber. Therefore, for photons with greater wavelengths, management in the rear side of the structure is required. The use of cluster-shaped NPs can lead to a significant change in optical absorption and is helpful for design of a cell with high photocurrent. On the other hand, a low-energy photon helps to create electron-hole pairs induced by the localized surface plasmonic effect of the NPs.

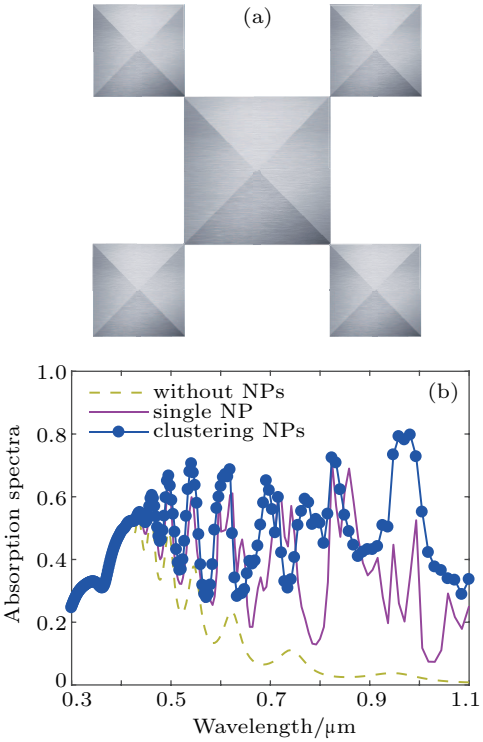


Fig. 3. Absorption spectra of a 400 nm ×400 nm ×400 nm silicon solar cell with cluster-shaped pyramidal Ag NPs at the backside compared with a cell without nanoparticles.

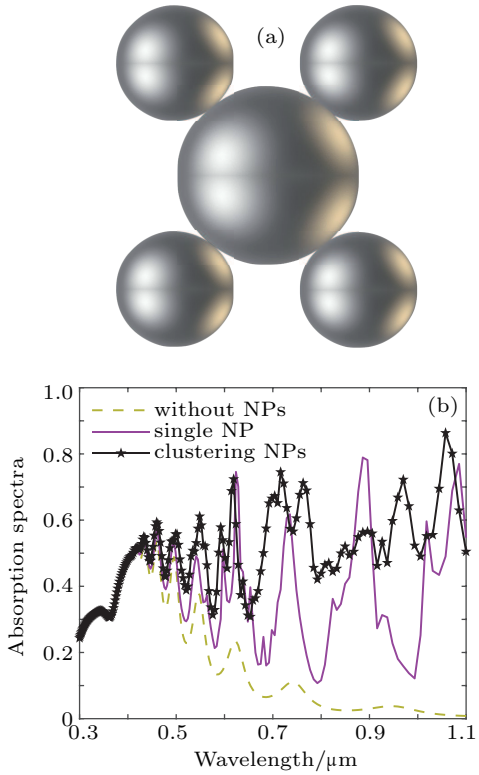


Fig. 4. Absorption spectra of a 400 nm×400 nm×400 nm silicon solar cell using clustering spherical-shaped Ag NPs at the backside, compared with a cell with one NP and without nanoparticles.

In the next step, an ultra-thin cell is designed using clustering conical-shaped NPs at its backside, as shown in Fig. 5(a). Figure 5(b) depicts its optical absorption spectrum and compares it with the absorption spectra of a cell with one

NP and without NPs. Their effect on light absorption can be seen clearly. As shown in this figure, absorption peaks at higher wavelengths are higher. It can be said that by clustering the nanoparticles, the absorption becomes uniformly high and more suitable in the desired wavelengths.

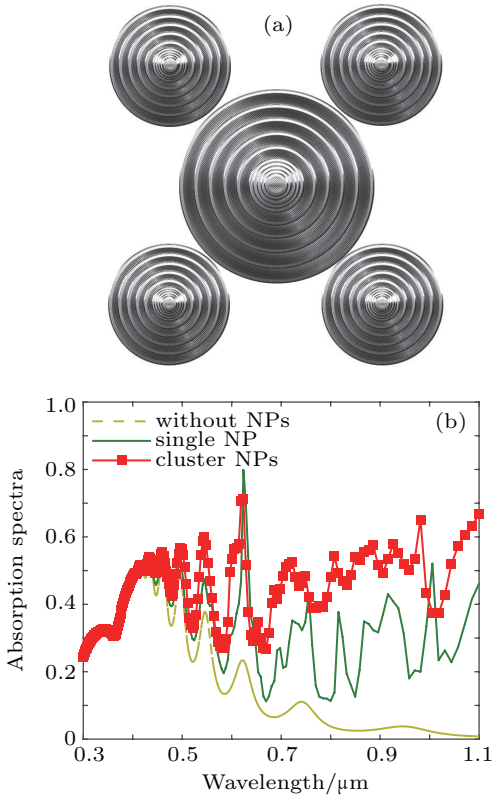


Fig. 5. Absorption spectra of a 400 nm×400 nm×400 nm silicon solar cell with cluster-shaped conical Ag NPs at the backside, compared with a cell with one NP and without NPs.

For the next step, a cell using cluster-shaped cylindrical NPs is simulated, as schematically shown in Fig. 6(a). Figure 6(b) shows the comparison of its absorption spectrum with a cell without nanoparticles and a cell with a single cylindrical-shaped nanoparticle.

To compare the role of each nano-cluster, here the comparison is made. The absorption spectra and hence the photocurrent of them are compared. The aim is to find which nano-cluster increases them significantly. Figures 7(a) and 7(b) show the absorption spectra of a silicon solar cell with clustering pyramidal, spherical, conical and cylindrical Ag NPs with the unit cell volume of $300 \times 300 \times 300$ and 400 nm ×400 nm ×400 nm, respectively. The photocurrent is a good measure for comparison. Therefore, the photocurrents of the cells with the aforementioned clustering nanoparticles are presented in Table 1.

As seen clustering nanoparticles improve the photocurrent more than non-clustering cases. Therefore, the clustering technique is the right candidate for further improvement in ultra-thin solar cells. It is important to mention that compared to the reference cell, the photocurrent enhancement is higher. These improvements are due to the plasmonic effects of nanoparticles.

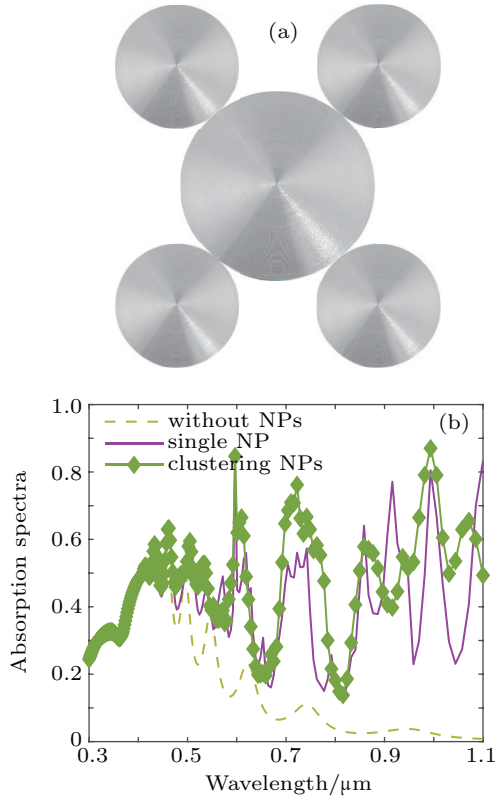


Fig. 6. Absorption spectra of a 400 nm×400 nm×400 nm silicon solar cell with cluster-shaped cylindrical Ag NPs at the backside compared with a cell without nanoparticles.

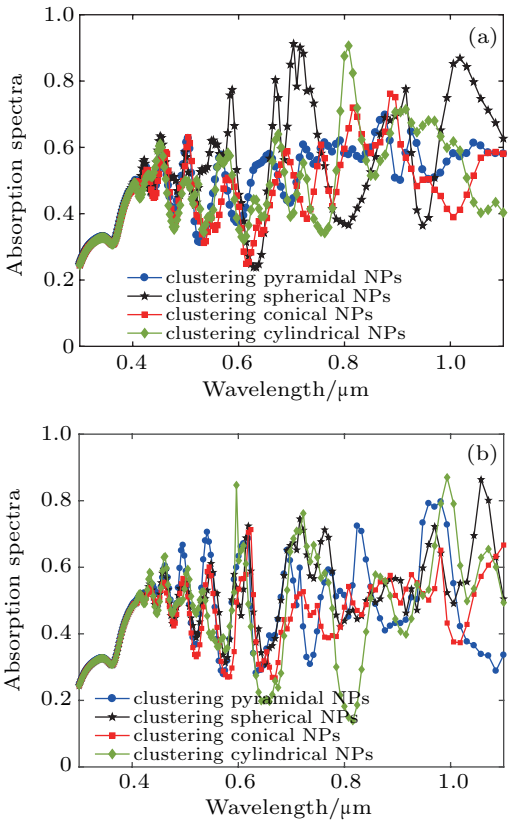


Fig. 7. Comparison the absorption spectra of a silicon solar cell with cluster-shaped pyramidal, spherical, conical and cylindrical Ag NPs (a) $300 \times 300 \times 300$ and (b) 400 nm×400 nm×400 nm.

Table 1. A comparison between the short circuit currents of different simulated structures.

Structure	Short circuit current/(mA/cm^2)			
The volume of a unit cell	300×300×300	300×300×400	400×400×300	400×400×400
Reference cell	5.3609	6.3209	5.4002	6.3672
A cell with clustering pyramidal NPs	23.043	23.921	22.041	21.427
A cell with one pyramidal-shaped NP	12.962	13.823	14.746	16.507
A cell with clustering spherical NPs	25.169	24.015	21.698	23.186
A cell with one spherical-shaped NP	16.178	17.186	15.450	16.901
A cell with clustering conical NPs	21.453	22.406	19.659	20.478
A cell with one conical-shaped NP	12.860	14.535	10.677	13.987
A cell with clustering cylindrical	22.292	22.998	18.967	21.243
A cell with one cylindrical-shaped NP	17.866	16.128	15.763	17.926

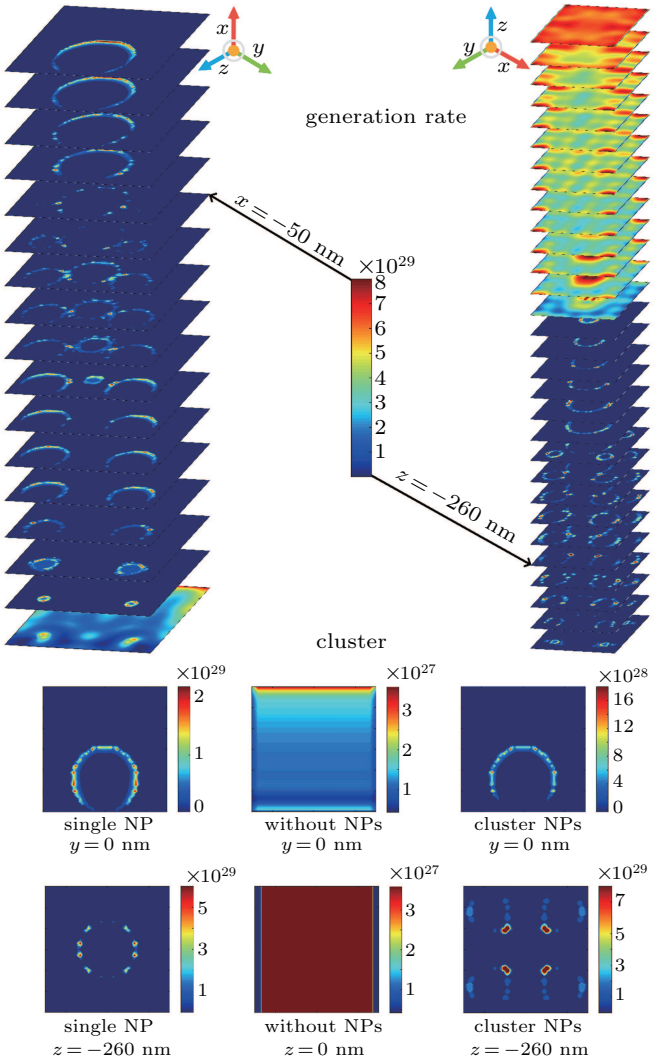


Fig. 8. Calculated generation rates for a cell without nanoparticles, a single spherical-shaped NP at the rear side and cluster-shaped spherical NPs at the rear side. Here x and y range from -0.15 to $+0.15$, z ranges from -0.3 to 0.

As mentioned above, the management of incident light for the wavelengths in the range of the visible and near-infrared range is used to improve the photocurrent of an ultra-thin film silicon solar cell. Resonant absorption of light energy by electron oscillations occurs under the condition of equality of the momentum vector of the surface plasmon and the projection of the photon momentum vector onto the interface of the media. That depends on the properties like refractive indices of the media, the frequency of incident light, the shape of nano-particles, etc. If the resonance conditions are met, then the intensity of the reflected light into absorber increases dramatically. The generation rate is one of the most important parameters of the solar cell, which gives us the number of electrons produced at each point in the device, due to the absorption of the photons. In Fig. 8, the optical generation rate is shown for clustering the spherical-shaped NPs. For more comparison, in Fig. 8, the cross section of the generation rates of the cells with single nanoparticle and without nanoparticles are presented. As can be seen, the generation rate for a cell without NPs is less than the others. As is shown, the generation rate in the cluster-shaped mode of NPs is better than that of a single nanoparticle. Images on the right were taken in the direction of the z-axis and the images on the left in the direction of the x-axis. As our results supported, clustering the nanoparticles significantly enhances the optical absorbance of the cell. Clustering such metal nanoparticles inside the active layer concentrates the electromagnetic field associated with an enhanced near-field scattering in the vicinity of the nanoparticles. It is concluded that using an array of nanoparticles in the form of clustering with the same volume of non-clustering nanoparticles, the higher the absorption is, the higher the photocurrent can be obtained.

4. Conclusion

In this research work, plasmonic effects in metal nanoparticles whose arrangement is in the form of clustering shape are used to design an ultra-thin silicon solar cell. First, a single pyramidal, spherical, conical, and cylindrical shaped nanoparticle in the backside of a thin absorber is simulated. Then, for further photocurrent enhancement, clustering pyramidal, spherical, conical, and cylindrical NPs is performed, and a further improvement in the absorption spectra and photocurrent is reported. The photocurrents of 20.478 mA/cm^2, 23.186 mA/cm^2, 21.427 mA/cm^2, and 21.243 mA/cm^2 are obtained for them, respectively. These values are 13.987 mA/cm^2, 16.901 mA/cm^2, 16.507 mA/cm^2,

and 17.926 mA/cm^2 for single nanoparticle cases, respectively. As a result, clustering causes further improvement in photocurrent.

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