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Investigation of hybrid Ge QDs/Si nanowires solar cell with improvement in cell efficiency

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In this paper, the structure of a high-efficiency solar cell is presented by using a combination of quantum dots of germanium arrays and silicon nanowires on a thin film silicon layer. Due to the low absorption coefficient of silicon, this type of solar cell does not have high efficiency. According to the capability of the quantum structure in absorbing the incident photons and the generation of electron-hole pairs, this structure is proposed. Moreover, nanowires as an appropriate suggestion are applied in our work aiming to improve light scattering and optical photon absorption for the generation of carriers. Both of the electrical and optical characteristics of the solar cell are calculated by using a finite-difference time-domain method. Owing to the change of the nanowire length and increasing the number of quantum dot in our work, maximum power absorption is achieved. The achieved results provide a considerable improvement in efficiency and short-circuit current density. The efficiency is improved up to 17.5% and the short-circuit current density in the active layer of thickness 1170 nm has been provided to be 42.6 mA/cm^2. The open circuit voltage for this cell is calculated to be 0.47 V. The achieved results provide a considerable improvement in efficiency and short-circuit current density in comparison with previously published method.

Keywords: nanowire, absorption, FDTD, hybrid structure, thin-film, cylindrical quantum dots.

1. Introduction

Although the first-generation single-junction silicon solar cells have achieved acceptable performance in recent years, they need to be further investigated due to the low absorption coefficient of silicon and its inability in the absorption of photons with energies lower than its band gap [1–3]. Several researches have been done to absorb photons having lower energy than the band gap using different structures. One of the proposed solutions is the use of quantum dots such as InAs and CdS, within the absorber layer [4]. Although solar cells that use quantum dots increase the absorption of light, the voltage of the open circuit is lower than that of the base cells without the quantum dots. There is a slight increase in current, but much larger decrease in voltage resulting in lower efficiency [5].

Another method to improve cell performance in absorbing photons and collecting effective carriers to produce photocurrent is using of nanowires which have a radius from 100 nm up to 2 μm [6]. To enhance the efficiency of the solar cells, reducing the surface and bulk recombination losses is very effective. By using materials with a band gap larger than the absorber layer such as GaP in the silicon structure, the surface recombination can be controlled [7]. Due to the fact that thin-film solar cells are low -cost and efficient, with an array of nanowires they have been used to reduce the bulk recombination [8]. The ability of absorbing the incident light in the cell and collecting the carriers, increases the cell efficiency. There are few materials such as GaAs with mentioned capabilities. The quality of materials used in nanowire structures plays a positive role in high efficiency.

One of the characteristics that shows the high quality of the material for use as an absorber layer is the absorption depth of light at the wavelengths of the optical spectrum. The layout of nanowires on the substrate is also useful in absorbing light. When the layout of nanowires is arranged as an array, the light absorption is decreased. In addition, the length of the light passway will increase if the nanowires are randomly distributed [9]. As HUA BAO and XIULIN RUAN have shown in [10], the absorption improvement in the structure with vertical nanowire without using the anti-reflection coating, is due to the enhancement of the light scattering in the cell. The smaller radius of the nanowires causes more light scattering and trapping in the cell.

Different hybrid structures and heterojunctions have been proposed to achieve mentioned goals [11]. Heterojunction structures used widely are *p*-type quantum dots such as PbS and *n*-type semiconductor with a large band gap like ZnO [12]. For extraction of carriers in these structures, layers with a thickness of 300 nm are required. In the case of the thickness of the quantum dot PbS that has the ability to extract full carrier is 1 μm [13]. In some structures, radial silicon *p*-*n* junction and silicon nanocrystalline quantum dots have been used aiming to reduce the recombination and optical losses with an efficiency of about 13% [8].

The InP nanopillar structure not only increases the cell efficiency of heterojunction structure and reduce the reflection of light, but also increases the length of light passway [14]. Although, the use of Ge quantum dots in the silicon structure leads to proper performance of the growth of silicon nanowire on silicon, it requires a temperature of about 450 degrees for initial growth which increases the cost of construction [15]. The temperature independence of the conductivity is the advantage of applying the silicon nanowire on a thin film silicon layer [16].

In this paper, we use the silicon nanowire composite structure on silicon and employ the geometric quantum dots arrays. In this structure, the placement of silicon nanowires on a substrate of the *p*-type silicon increases the cell efficiency by reducing the carrier collecting losses. The array of cylindrical quantum dots on top of the nanowires improves the absorption of light in visible light wavelengths and increases the maximum optical power absorption P_{abs}. One of the advantages of simultaneous use of quantum dots and nanowires in this structure is an increase in the absorption and electron-hole pairs generation rate inside the cell [17] as it will be shown in Figs. 10**a** and 10**b**.

The reduction of optical losses and recombination surface in this structure result in an efficiency of 17.5% for simulated cells. In the next section, the proposed structure is described in detail, and then the simulation results are analyzed and discussed. The conclusion is presented in the final section.

2. The structure of solar cell

In this paper, an optical and electrical simulation about Ge QD/Si nanowire solar cells was investigated to explore the properties of the optimal structure for this cell. First, the influence of the length of Si nanowire on the electrical characteristic of solar cell is analyzed. Second, to further investigate optical and electrical characteristic of solar cell, maximum absorption power of cell with increasing number of QDs above the nanowire is evaluated by using a finite-difference time-domain method. Finally, the influence of the shape of QDs is validated by changing cylindrical QDs to pyramid QDs.

Figure 1 shows the schematic of the hybrid proposed structure for solar cell, which is composed of nanowires with an initial length of 400 nm and their center-to-center distance (pitch) of 150 nm on silicon substrate with a thickness of 500 nm.

The radius of cylindrical quantum dots is 10 nm and the array is decorated with center-to-center distance (pitch) of 30 nm at a distance of 150 nm on top of nanowires. The specification of the initial thickness, the type and their amounts of materials used are presented in Table 1. The initial thickness as shown in Table 1 to improve hybrid

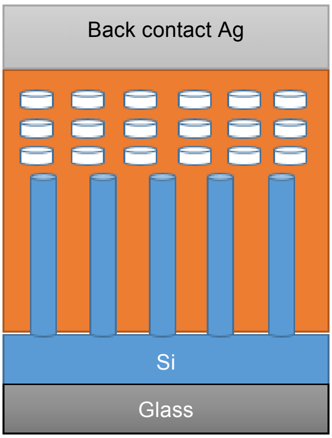

Fig. 1. The schematic of the proposed solar cell.

Table 1. Details of proposed structure.

Material	Thickness	Radius	Pitch
Glass	20 nm	–	–
Si	500 nm	–	–
Nanowire Si	400 nm	60 nm	150 nm
Quantum dot Ge	–	10 nm	30 nm
Back contact Ag	20 nm	–	–

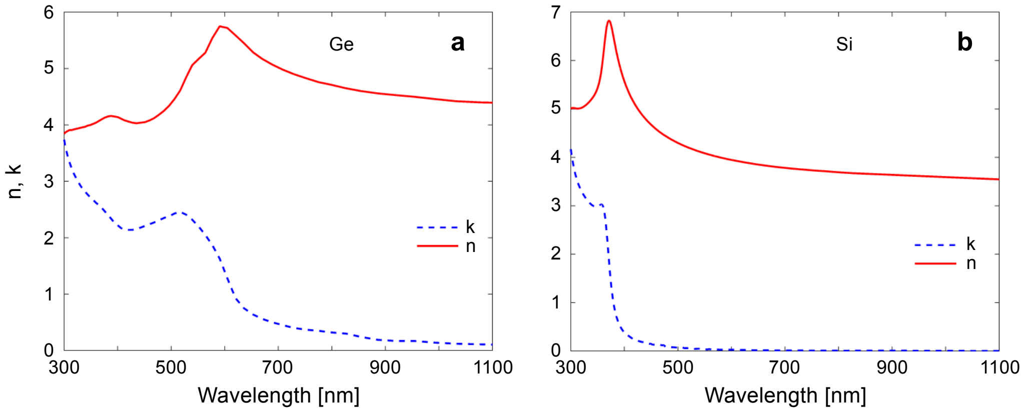

Fig. 2. Refractive index and extinction coefficient of Ge (**a**) and Si (**b**) used in the simulation [18].

structure is 500 nm, then by using nanowires and quantum dots the best efficiency and short-circuit current is achieved at a thickness of less than 1 μm. Figure 2 shows the refractive index of Ge and Si used in this simulation. The simulation of proposed cell was carried out under the standard AM1.5 solar power spectrum without concentrating the light. The simulation is repeated several times for optical stability. To simulate optical properties of the solar cell, we computed total optical absorption as follows [3]:

$$A(\lambda) = \frac{1}{2}\int \omega(\lambda)\left|E_{x,y,z,\lambda}\right|^2 \varepsilon(\lambda)\,\mathrm{d}V \tag{1}$$

where $\omega(\lambda)$ is the angular frequency, $E_{x,y,z,\lambda}$ is the electric field intensity, and $\varepsilon(\lambda)$ is the imaginary part of the permittivity. The optical current density J_L is calculated by integrating the total optical absorption multiplied by solar irradiance spectrum over the wavelength range of 300–1100 nm as [3]

$$J_L = q\int_{300}^{1100} \frac{\lambda}{hc} A(\lambda) F(\lambda)\,\mathrm{d}\lambda \tag{2}$$

where q is the charge, h is the Planck constant, c is the speed of light, and $F(\lambda)$ is the intensity of AM1.5G solar spectrum. The current density for electrons and holes is solved by using drift-diffusion equations [3]:

$$J_n = q\mu_n n E + qD_n \nabla_n \tag{3}$$

$$J_p = q\mu_p p E - qD_p \nabla_p \tag{4}$$

where J_n (J_p) is the electron (hole) current density, μ_n (μ_p) is the electron (hole) mobility, D_n (D_p) is the electron (hole) diffusion constant, E is the electric field, and n (p) is the electron (hole) density. The continuity equations are required for calculation of concentrations of electrons and holes [3]:

$$\frac{\delta n}{\delta t} = \frac{1}{q}\nabla \cdot J_{\mathrm{n}} - R_{\mathrm{n}} + G_{\mathrm{L}} \tag{5}$$

$$\frac{\delta p}{\delta t} = \frac{1}{q}\nabla \cdot J_{\mathrm{p}} - R_{\mathrm{p}} + G_{\mathrm{L}} \tag{6}$$

where R and G_{L} are the recombination and optical generation rate, respectively. The EM field could be calculated when the Poisson's equation is solved [3]:

$$\nabla^2 V = \frac{q(n - p + N_{\mathrm{A}}^{-} - N_{\mathrm{D}}^{+})}{\varepsilon} \tag{7}$$

where V is the electrostatic potential, N_{A} and N_{D} are the acceptor and donor concentrations. The J-V characteristic of hybrid solar cell can be expressed by the following equation:

$$J = J_{\mathrm{sat}}\left(\exp\left(\frac{qv}{nk_{\mathrm{B}}T}\right) - 1\right) \tag{8}$$

where J_{sat} is the saturation current density, n defines the ideality factor of p-n junction, k_{B} is the Boltzmann constant, T and q are the absolute temperature and the electronic charge (1.6×10^{-19} C), respectively [19]. The values of the parameters used in simulations are listed in Table 2.

The parameters which are effective in the simulation of the structure are the radius of quantum dots, number of quantum dots, pitch of quantum dots array and their shape. Moreover, the length of nanowires, the pitch and radius of nanowire arrays are affective on solar cell characters.

In this simulation, the pitch and radius of nanowires were fixed at 150 and 60 nm, respectively, so that the quantum dot radius and pitch of its array were fixed at 10 and 30 nm, respectively. The active layer thickness included QDs and Si nanowire is

Table 2. Parameters used in the simulation of hybrid solar cell.

Material	Parameter	Description	Values [20, 21]
Si	E_{g}	band gap energy	1.12 eV
	φ	work function	4.59 eV
	$\mu_{\mathrm{n}}, \mu_{\mathrm{p}}$	electron, hole mobility	99 $\mathrm{cm^2\,V\,s^{-1}}$
	ε	dielectric permittivity	11.9
	$N_{\mathrm{A}}, N_{\mathrm{D}}$	acceptor, donor concentration	5×10^{18} $\mathrm{cm^{-3}}$
	τ	carrier lifetime	4 ns
	m_{e}	effective mass	0.49
Ge	E_{g}	band gap energy	0.66 eV
	m_{e}	effective mass	0.28
	φ	work function	4.5 eV

changed to calculate the power absorption. The result of optical and electrical characteristic of this structure is discussed in the following Section.

3. Results and discussion

First, the simulation is performed to find the optimal thickness of the active layer. In the case of a solar cell with no quantum dots and nanowires, when the thickness increases, the recombination increases and the open circuit voltage decreases. But when the nanowire is used in the structure, changing the thickness of the active layer also changes the length of the nanowire, resulting in an optimal length of nanowires, slight increase will be obtained in the open circuit voltage. Also according to the results in the previous researches, the relationship between the change in the length of the nanowire and the open circuit voltage is not linear [22, 23]. Table 3 shows the photovoltaic properties of hybrid structure with one layer quantum dots above nanowires and various lengths of nanowires from 400 to 1200 nm. In this case, since the array decoration of the silicon nanowires makes it possible to separate all the electron-hole pairs generated in the depletion region as free carrier, the increase in the thickness of the active layer (increase in length of nanowire) improves the short-circuit current. In this condition, since the resistance of the transfer of charge in silicon nanowires increases, the fill factor decreases.

As shown in Table 3, the open circuit voltage and efficiency reach maximum at the absorber layer thickness of 970 nm. In addition, the highest amount of short-circuit current is obtained at 1170 nm. In this state, the optimal length of nanowires for the structure is 800 nm. In Fig. 3, the results of the conditions according to Table 3 are shown. In the following, the electrical and optical characteristics are presented for different cell types.

Moreover, the effect of increasing in the quantum dots on the optical and electrical characteristics of the structure is investigated. The optimum length of nanowires is kept constant and the number of layers of the quantum dots is increased to achieve an optimal amount for it. In this simulation, cylindrical quantum dots arrays are used that have a radius of 10 nm with center-to-center distance (pitch) of 30 nm at a distance of 150 nm above the nanowires. By increasing the number of cylindrical quantum dots layers up to 4 layers, the optimal mode is calculated. Therefore, the highest efficiency is achieved in the placement of 3 layers of quantum dots on top of the nanowires. As depicted in Table 3, although the absorbed power and current reach a maximum in

Table 3. Comparison of the results by changing the length of the nanowires.

Thickness of active layer [nm]	V_{oc} [V]	J_{sc} [mA/cm^2]	$\eta_{\%}$
570	0.43	34.15	13.54
770	0.43	37.6	14.6
970	0.453	39.9	16.2
1170	0.41	42.12	15.3
1370	0.407	40.3	14.24

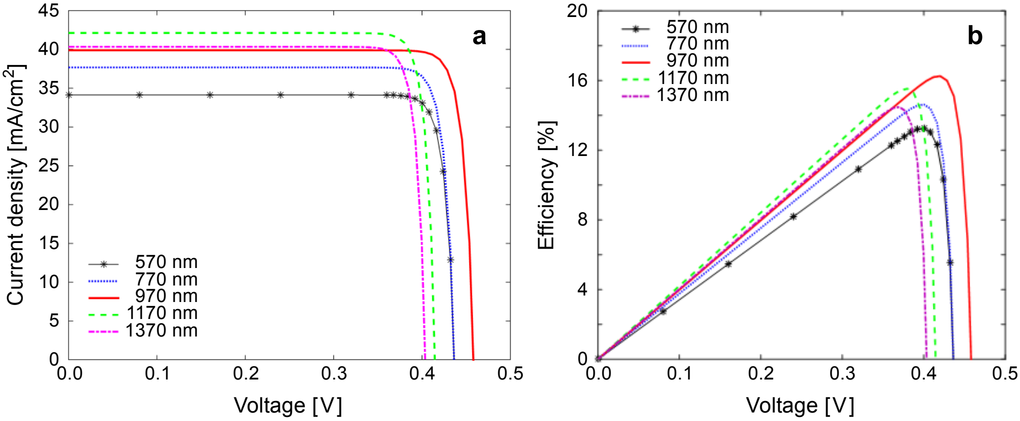

Fig. 3. Current density-voltage characteristics (**a**) and efficiency (**b**) of hybrid structure by changing the length of the nanowires.

4-layer mode, owing to the decrease of the open circuit voltage, the efficiency is decreased. The results of the condition according to Table 4 are shown in Figs. 4 and 5. In Figure 5, the absorbed power in the two cases of 3 layers and 4 layers of quantum dots at the wavelengths between 600 and 800 nm has the highest value, which results in the highest value for current density in the 4 layers case.

T a b l e 4. The result of changing the number of QDs layers above the nanowire (P_{abs} – maximum power absorption per unit).

Number of QDs layers	V_{oc} [V]	J_{sc} [mA/cm^2]	$\eta_{\%}$	P_{abs}
1	0.462	39.9	16.20	0.803
2	0.467	40.1	16.54	0.826
3	0.47	42.3	17.50	0.838
4	0.46	42.6	17.36	0.846

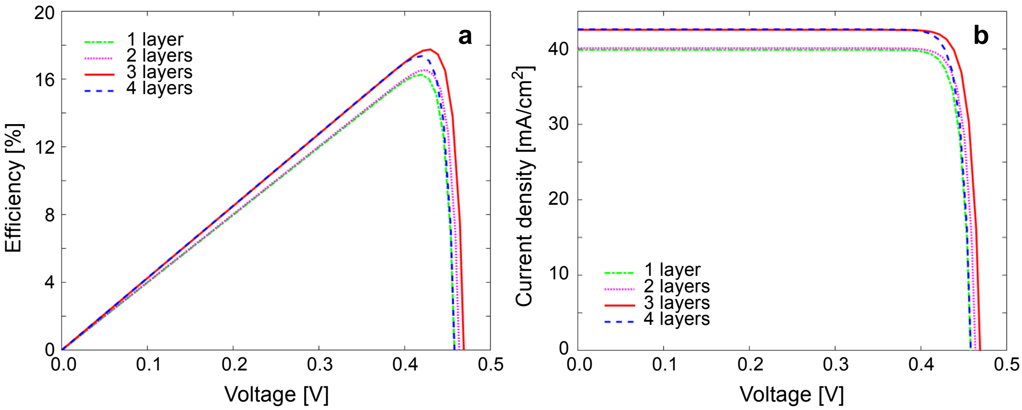

Fig. 4. Efficiency (**a**) and current density (**b**) with the changing number of QDs layers above nanowires.

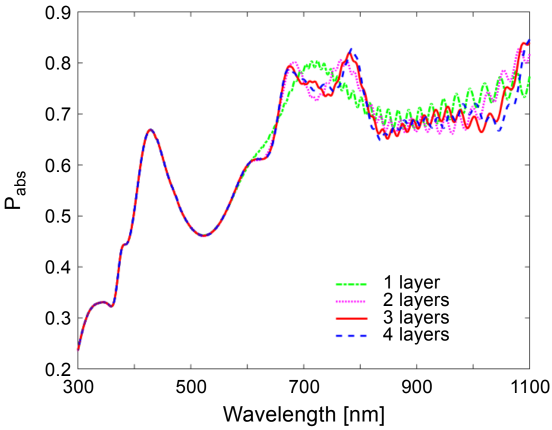

Fig. 5. Power absorption per unit with the changing number of QDs layers above nanowires.

In mentioned structure, the cell efficiency and the short-circuit current are improved by using cylindrical quantum dots of germanium with a radius of 10 nm decorated in an array with pitch of 30 nm. The use of germanium quantum dots allocated above the silicon nanowires increases quantum efficiency, and consequently, enhances the electron-hole pairs generation rate. When the electron is in Si layer, the impressive hole of Ge exists simultaneously [24]. In the following, the different states of quantum dots and changes in the shape of the dots above the nanowire are investigated. The absorption of light according to the incident light angle for various shapes of quantum dots is depicted in Fig. 6.

As shown in Fig. 6, the cylindrical quantum dots have more absorption than the pyramidal ones. In next investigation, this optimal structure (3 layers of quantum dots

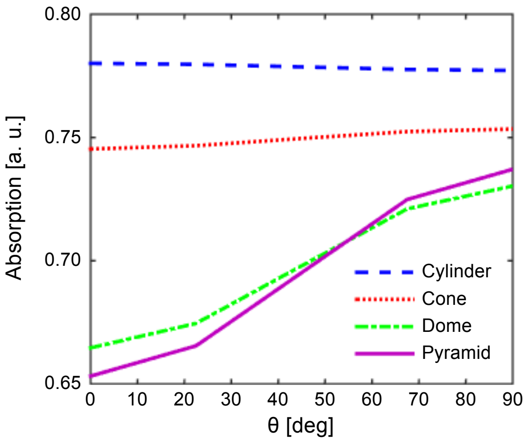

Fig. 6. Quantum dots absorption *vs.* incident light angle.

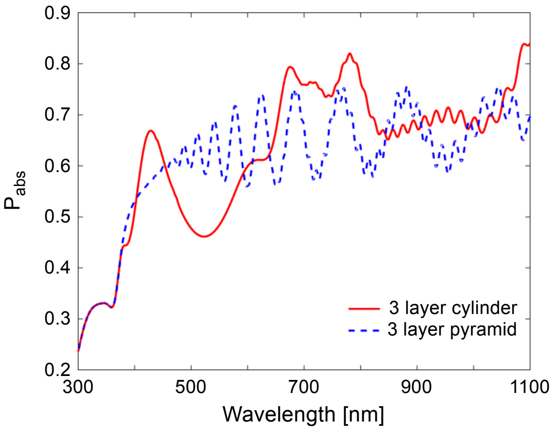

Fig. 7. Power absorption of hybrid structure.

and nanowires with a length of 800 nm) is simulated to evaluate the changes in the electrical and optical characteristics of the cell with respect to the change in the shape of the quantum dots in two states of the cell with pyramidal and cylindrical dots.

As shown in Fig. 7, the maximum power of the light absorption in a cell with three layers of cylindrical quantum dots has a good improvement than pyramidal quantum dots aiming to achieve high current and efficiency. As shown in Fig. 6, the absorption of cylindrical quantum dot is larger than the pyramid, and is less dependent on the angle of light, so the absorbed power has also increased, which according to

$$\mathrm{QE}(\lambda) = \frac{P_{\mathrm{abs}}(\lambda)}{P_{\mathrm{in}}(\lambda)} \tag{9}$$

leads to an increase in quantum efficiency. Finally, according to

$$J_{\mathrm{sc}} = q\int \frac{\lambda}{hc}\mathrm{QE}(\lambda)\, I_{\mathrm{AM1.5G}}(\lambda)\,\mathrm{d}\lambda \tag{10}$$

the short-circuit current density has increased, due to the fact that the open circuit voltage is constant when the efficiency has been increased.

Optical and electrical results are shown in Figs. 8**a** and 8**b**. Also in Figs. 9 and 10 as previously explained, we compare the absorption power and generation rate in conventional Si solar cell without nanowires and with them, respectively.

The results associated with Figs. 7 and 8 are shown in Table 5. Due to a variety of the structures and materials used in solar cells, it is usually difficult to compare fairly between our results with previously published structures. However, the overall performance of the proposed method could be compared to some published methods regarding nanowire solar cells.

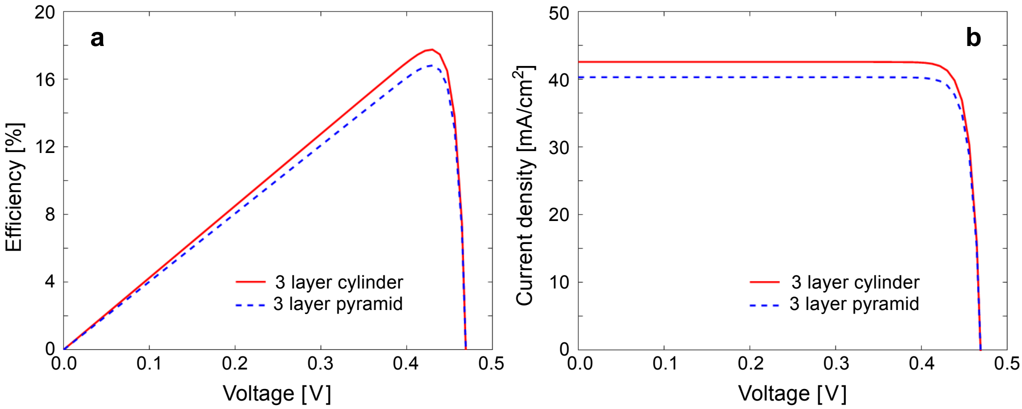

Fig. 8. Efficiency (**a**), and current density-voltage characteristic (**b**) for different shapes of quantum dots.

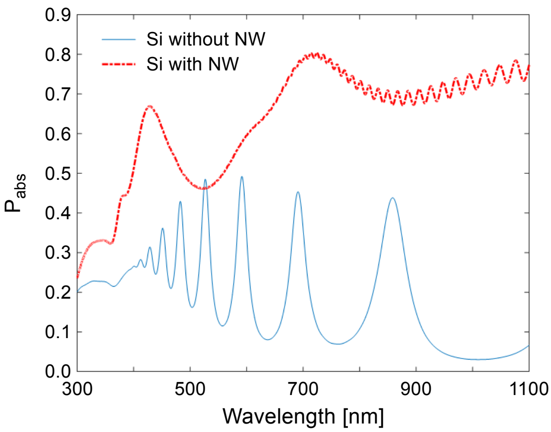

Fig. 9. Comparison of the absorption power in conventional Si solar cell without and with nanowires.

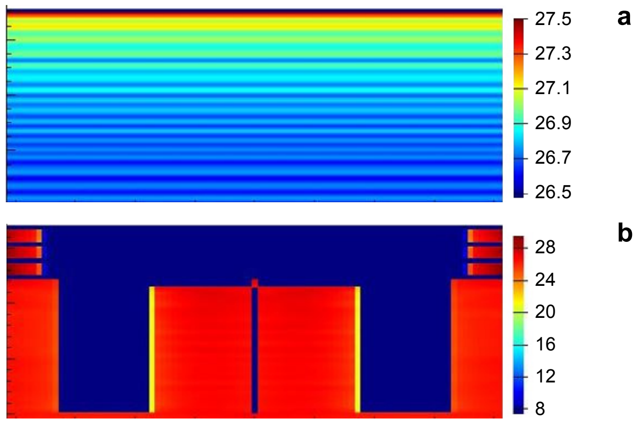

Fig. 10. Generation rate in conventional Si solar cell without (**a**) and with (**b**) nanowires.

Table 5. Photovoltaic characteristics of hybrid solar cells with different shape of QDs.

QDs type	V_{oc} [V]	J_{sc} [mA/cm^2]	$\eta_{\%}$
Cylinder	0.47	42.3	17.5
Pyramid	0.47	40.3	16.75

The simulation has been applied to nanowire solar cell investigated in [25]. It has been noted that the structure is only investigated optically, and it evaluates in the low wavelength range. These results in comparison with XIN YAN *et al.* have shown higher efficiency and short-circuit current by 4% and 14%, respectively [11].

4. Conclusion

In conclusion, both of optical and electrical simulation was investigated to calculate the optimized design requirements to improve optical and electrical characteristics of Ge QD/Si nanowires solar cells. It is found that absorption and efficiency are further optimized by using germanium quantum dots and silicon nanowires on a silicon substrate, with the adequate number of cylindrical quantum dots, light absorption and energy absorbed by the nanowires increase. Moreover, the nanowires that are placed vertically on silicon increase the light scattering, which results in more light absorption, the electron-hole pairs generation rate and the cell efficiency. Using a thin film of silicon, and changing the thickness of the active layer, the surface and bulk recombination are decreased. The use of silicon nanowires, quantum dot arrays and the adjustment of the placement of them have increased light trapping and have reduced the spectral and optical losses. With changes in the thickness of the active layer and length of nanowire, the highest efficiency and open circuit voltage at 970 nm were obtained to be 17.5% and 0.47 V, respectively. The maximum short-circuit current is provided 42.6 mA/cm^2 in the active layer thickness of 1170 nm with 4 layers of cylindrical quantum dots. The optical and electrical characteristics when use cylindrical quantum dots in comparison with pyramidal shape of quantum dots are enhanced. In this paper, with an appropriate change in the length of the nanowire and the number of layers of the quantum dots, resulting in the improvement of the active layer thickness, the efficiency and current increased to 17.5% and 42.3 mA/cm^2, respectively.

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