

Analysis of poly-Si thin film p^+-n-n^+ homojunction solar cell and heterojunction solar cell with and without a thin $\mu\text{c-Si}$ layer at the interface of $a\text{-Si}$ and poly-Si layers

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Abstract. In this study, new possibilities for higher efficiency poly-Si thin film solar cells are investigated using MEDICITM device simulator. The poly-Si p^+-n-n^+ thin film solar cell with a thin $a\text{-Si}$ p^+ layer is found to have higher efficiency than the homojunction p^+-n-n^+ cell. Further improvement in efficiency of the heterojunction p^+-n-n^+ cell is achieved by introducing a thin $\mu\text{c-Si}$ layer at the interface of $a\text{-Si}$ emitter and poly-Si absorber layers. The $\mu\text{c-Si}$ layer at the interface is found to reduce the recombination losses at the interface and improved the fill factor and efficiency of the cell. The photovoltaic parameters of the cell and the absorber layer thickness for optimum efficiency are highly influenced by grain size and passivation at the grain boundary.

PACS. 78.30.Fs III-V and II-VI semiconductors – 78.55.Cr III-V semiconductors – 85.30.De Semiconductor-device characterization, design, and modeling

1 Introduction

The polycrystalline silicon (poly-Si) thin film solar cells are most promising due to high efficiency, high stability, low-cost and reliability. This emerging technology combines the advantages of crystalline Si (c-Si) with thin film approach and is not yet as mature as amorphous Si ($a\text{-Si}$) or c-Si technologies, but has a lot of scope for development. The small grain sizes and the recombination at the grain boundary prevent these cells from achieving higher efficiencies [1–4]. A deeper understanding of the effect of the passivation of the grain boundaries and the grain sizes on the cell performance is needed for developing high efficiency poly-Si solar cells. The heterojunction solar cells consisting of a poly-Si base and having a very thin $a\text{-Si}$ emitter can attain a higher open circuit voltage (V_{oc}) than the homojunction solar cells [5,6]. The heterojunction solar cells created by depositing thin $a\text{-Si}$ layer on top of c-Si substrate gained much interest due to its potential to achieve very high efficiencies [7]. However, there is a large opportunity for improving the cell performance and various factors that influence the cell performance can be very conveniently investigated by computer simulations. In this study, we used MEDICITM (Version 2000.2; Avant! Corporation, Fremont, CA), which is a two-dimensional device simulator, to simulate the electrical behaviour and the performance of a heterojunction poly-Si thin film solar

cell having an $a\text{-Si}$ emitter layer. The effect of introducing a thin layer of microcrystalline Si ($\mu\text{c-Si}$) between the $a\text{-Si}$ and the poly-Si layers on the efficiency of the heterojunction thin film solar cell is investigated. It is found that this modified cell structure could result in a higher efficiency. We also analyzed the effect of the grain size and the degree of passivation of the grain boundary on the photovoltaic parameters and the absorber layer thickness, for optimum efficiency of the homojunction poly-Si cell.

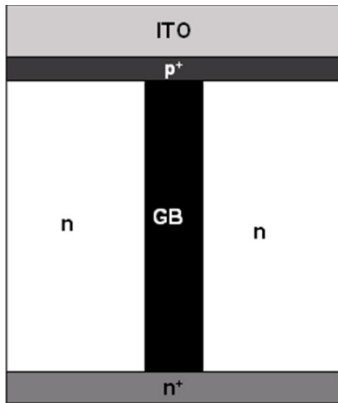
2 Simulation model

We used the Shockley-Read-Hall and the Auger recombination models, the concentration dependent lifetimes and the low field mobility model in our investigation. The photogeneration model consisting of a ray tracing algorithm is used to calculate the transmission and absorption of light in the bulk, and reflection and refraction at the interfaces. The p^+-n-n^+ cell considered here operates under the global standard solar spectrum (AM 1.5) illumination with 100 mW/cm² total incident power density and the light intensity for each wavelength is calculated in the wavelength range of 0.2 to 1 μm . A structure consisting of glass/ITO/poly-Si p^+-n-n^+ /Al in which light enters through the p^+ layer is considered as the model solar cell for simulation. A columnar-shaped structure of poly-Si thin film is assumed in this study and a 0.01 μm wide

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Table 1. The input parameter values for the simulation of poly-Si p^+-n-n^+ solar cell (electrical parameters are for the absorber layer).

Parameter	Unit	Value
ITO layer thickness	nm	60
p^+ -layer thickness	nm	30
n^+ -layer thickness	nm	60
Mobility gap, E_g	eV	1.1
Effective density of states N_c, N_v	cm^{-3}	1×10^{19}
Density of acceptor-like tail states at $E_t = E_c$	$\text{cm}^{-3} \text{eV}^{-1}$	1.2×10^{18}
Density of donor-like tail states at $E_t = E_v$	$\text{cm}^{-3} \text{eV}^{-1}$	2×10^{18}
Density of acceptor-like deep-gap states at $E_t = E_c$	$\text{cm}^{-3} \text{eV}^{-1}$	1.2×10^{16}
Density of donor-like deep-gap states at $E_t = E_v$	$\text{cm}^{-3} \text{eV}^{-1}$	4×10^{16}
Free electron's mobility, μ_n	$\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$	150
Free hole's mobility, μ_p	$\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$	50
Electron life time	μs	0.01
Hole life time	μs	0.1
Transmittance of glass/ITO	–	0.9
Reflectivity of n^+ /metal contact	–	0.9
Surface recombination velocity	cm s^{-1}	10^7


Fig. 1. The rectangular shaped grain boundary model used in this simulation.

rectangular shaped grain boundary is inserted between the two single-crystalline regions in the absorber layer (Fig. 1) that has a very short carrier lifetime (1×10^{-10} s). A carrier lifetime of 1×10^{-6} s is considered for the intra-grain regions. The grain boundaries are more or less passivated with three values of interfacial recombination velocities of 10^2 cm/s, 10^4 cm/s and 10^6 cm/s. We assumed that the trap states are localized at the grain boundaries in the poly-Si film and the density of states at the grain boundaries consisted of donor-like and acceptor-like states. The total density of states for carrier trap is thus expressed by $g(E) = gD(E) + gA(E)$, where $gD(E)$ and $gA(E)$ are the densities of states for donor-like and acceptor-like states, respectively, and E is the energy. The same distribution of the energy band gap states in the grain boundary of the poly-Si as in reference [8] is assumed in this work.

The solar cell is set to $10 \mu\text{m}$ wide and $1 \mu\text{m}$ deep in the z -direction and layer thicknesses of 30 and 60 nm for p^+ – and n^+ – layers respectively are used, while absorber layer thickness is varied from $1 \mu\text{m}$ to $6 \mu\text{m}$. We also assumed flat interfaces for this simulation study. For the so-

lar cell structure with the heterojunction, the p^+ emitter layer consisted of a -Si layer of 10 nm. The same parameters, which we have used in our earlier work [9], have been considered for a -Si p^+ layer in this simulation study also. The concentrations of p^+ , n^+ and n -type dopants are assumed as $1 \times 10^{19} \text{ cm}^{-3}$, $5 \times 10^{19} \text{ cm}^{-3}$, $1 \times 10^{15} \text{ cm}^{-3}$. For improving the performance of the heterojunction poly-Si cell with a -Si emitter, we introduced a thin layer of μc -Si at the interface of a -Si and poly-Si layers and the performance was simulated. The parameters considered for μc -Si are similar to that for poly-Si except the band gap which is considered as 1.4 eV and the density of defect states in the band gap that is one order higher than that of poly-Si material. A grain size of $0.05 \mu\text{m}$ is set for the μc -Si layer. The structural, electrical and optical parameters used for simulating the cell performance are shown in Table 1, which are adopted from literature [8,10–12].

3 Result and discussion

3.1 The poly-Si p^+-n-n^+ homojunction cell

At the outset, we analyzed the effects of the absorber layer thickness and the grain size on the performance of the poly-Si p^+-n-n^+ homojunction cell. Figure 2 shows the dependence of short circuit current density (J_{sc}), open circuit voltage (V_{oc}) and fill factor (FF) on the absorber layer thickness for different grain sizes of $0.1 \mu\text{m}$, $1 \mu\text{m}$ and $10 \mu\text{m}$. In this case, the grain boundary is assumed to be well passivated. It is obvious (Fig. 2) that the photovoltaic parameters are influenced considerably by the grain size and V_{oc} is the most affected. This is because the decrease in the grain sizes severely increases the recombination at the grain boundaries and heavily increases the diode current, which in turn adversely affects the V_{oc} . There is no appreciable difference in the J_{sc} for the three grain sizes upto an absorber layer thickness of $2 \mu\text{m}$. However, for the smaller grain sizes, significant difference in J_{sc} is observed

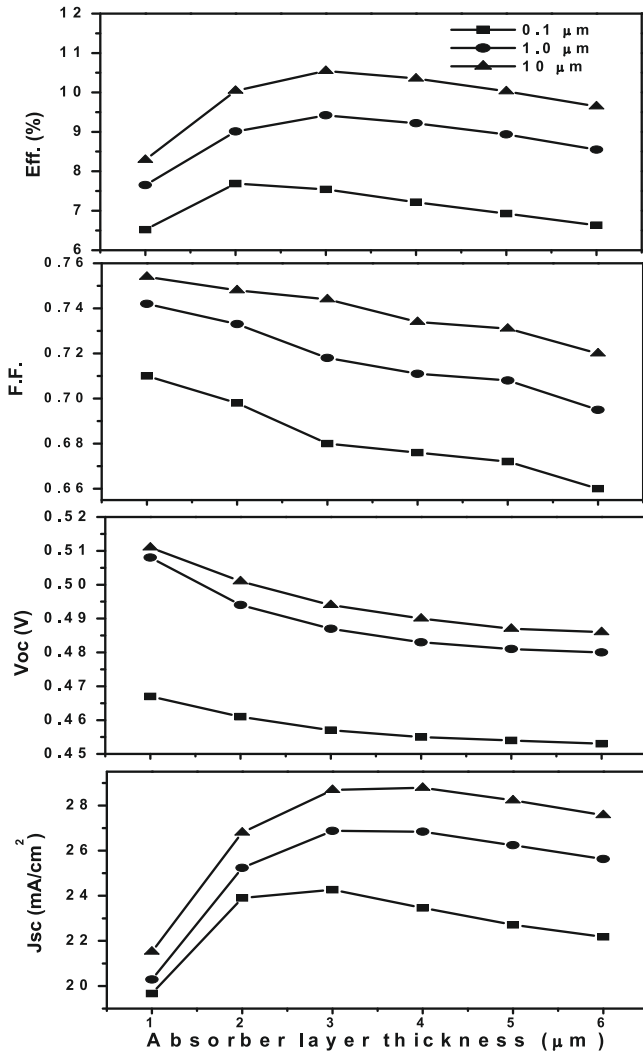


Fig. 2. The dependence of calculated photovoltaic parameters on n -doped absorber layer thickness of the homojunction $p^+ - n - n^+$ poly-Si cell with 0.1, 1, and 10 μm grain sizes.

when the absorber layer thickness is more than 2 μm . For 10 μm and 1 μm grain sizes, the optimum value of J_{sc} is obtained when the absorber layer is thicker (3 μm), whereas, for the small grain size of 0.1 μm , the optimum J_{sc} is obtained for a thinner (2 μm) absorber layer. This is because the overall defects in the material increases as the grain size decreases and J_{sc} increases with the increase in the absorber layer thickness up to equilibrium between grain size and layer thickness. The calculated optimum efficiencies for 10 μm , 1 μm , and 0.1 μm grain sizes are 10.545%, 9.42% and 7.69%, respectively. About 20% decrease in efficiency is observed when the grain size is decreased from 1 μm to 0.1 μm as against 10% decrease in efficiency when the grain size is reduced from 10 to 1 μm .

The influence of the grain boundary passivation on the cell efficiency is investigated by considering well passivated, partially passivated and least passivated grain boundaries and the calculated efficiencies as a function of the absorber layer thickness for the grain sizes of 0.1 μm ,

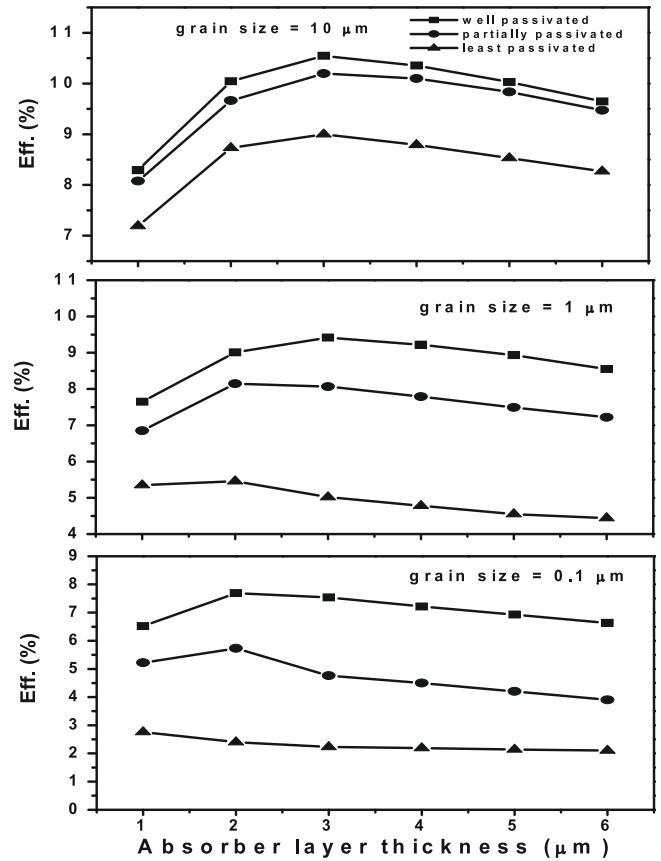


Fig. 3. The dependence of calculated efficiency of the homojunction $p^+ - n - n^+$ poly-Si cell on the degree of grain boundary passivation for 0.1, 1, and 10 μm grain sizes.

1 μm and 10 μm are shown in Figure 3. A recombination velocity of 10^2 cm/s for well passivated, 10^4 cm/s for partially passivated and 10^6 cm/s for least passivated grain boundaries are considered. For the 10 μm grain size, the cells with the well passivated and the partially passivated grain boundaries showed only a smaller difference in efficiencies for all values of the absorber layer thicknesses, but the cell with the least passivated grain boundary showed much lower efficiency. As the grain size is decreased, the differences between efficiencies of cells with the three passivation conditions are found to increase (Fig. 3), which indicated that the absorber layer thickness needed for optimum efficiency depends not only on grain size but also on the passivation conditions. Furthermore, for the 10 μm grain size, a 3 μm absorber layer is needed for achieving optimum efficiency for all the three passivation conditions. For the 1 μm grain size, optimum efficiency is obtained with 3 μm absorber layer for the well passivated grain boundary, whereas, for the partially and the least passivated grain boundaries, 2 μm absorber layer is needed for obtaining optimum efficiency. For the 0.1 μm grain size, the optimum efficiency for the well passivated and the partially passivated grain boundaries is obtained by using a 2 μm absorber layer, whereas, with the least passivated grain boundary, only 1 μm absorber layer is required for optimum efficiency.

Above results reveal that poly-Si thin film layers with well passivated grain boundaries and large grain sizes are required for achieving higher efficiency solar cells. Larger grain sizes can be obtained by using high temperature deposition processes, which results in highly expensive solar cells. However, lack of hydrogen at high temperatures can lead to weakly passivated grain boundaries, which leads to lower efficiencies. On the other hand, the inexpensive low temperature deposition processes can result in thin films with higher efficiencies due to well passivated grain boundaries, despite the small grain sizes.

3.2 The poly-Si p^+-n-n^+ heterojunction cell with a -Si emitter layer

The main difficulty in improving the conversion efficiency of the poly-Si solar cells is the relatively low V_{oc} obtained. It has been widely accepted that the efficiency or V_{oc} of the poly-Si solar cells are limited by the grain size of the layer and by the number of active grain boundaries. In order to increase V_{oc} by reducing the recombination velocity, several techniques for passivation of grain boundaries have been used. These techniques include: more efficient hydrogenation by shifting the chemical equilibrium between hydrogen passivation and defect formation [13], manipulating the crystal orientation of adjacent grains during growth so that it correlates with coincidence-site lattice theory [14–17], and more intentional dopant segregation to surround the grain boundaries with highly doped region [18]. Fabricating the heterojunction cells with a thin a -Si emitter layer on mullite ceramic substrate also can result in higher V_{oc} for fine-grained poly-Si thin film solar cells [19,20]. When a wide band gap a -Si emitter layer is used in the poly-Si heterojunction thin film cells, most of the photons are transmitted to the absorber layer, where the band gap is smaller and the optical generation rate is much higher. If the concentration of the interface states at the heterojunction is at acceptable levels, the carrier generation in the absorber layer will be higher, where the built-in field is high and the recombination rate is lower. In the case of the homojunction poly-Si thin film cell, this type of control of the carrier generation profile is impossible and the carrier collection efficiency will be lower than that of the heterojunction poly-Si thin film cell.

In this study, simulations are carried out to analyze the performance of the poly-Si p^+-n-n^+ heterojunction cell with a -Si emitter layer and it is found that this cell showed a better performance than the poly-Si p^+-n-n^+ homojunction cell (Tab. 2). For this analysis, we considered the poly-Si thin film solar cell with well passivated grain boundary discussed in Section 3.1, and with a -Si p^+ emitter layer of 15 nm. For the grain size of 0.1 μm , a conversion efficiency (η) of 8.24% is obtained with $V_{oc} = 0.49$ V, $J_{sc} = 24.60$ mA cm^{-2} , and $FF = 0.684$. The photovoltaic parameters obtained for the homojunction poly-Si cell having a similar device structure are: $\eta = 7.69\%$, $J_{sc} = 23.9$ mA cm^{-2} , $V_{oc} = 0.461$ V, $FF = 0.698$. The $J - V$ characteristics of these two cells are shown in

Table 2. The simulated results obtained for the homojunction and the heterojunction p^+-n-n^+ poly-Si solar cells for different grain sizes.

Grain size (μm)	Emitter type of the cell	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF	η (%)
0.1	Heterojunction	24.60	0.49	0.684	8.24
	Homojunction	23.90	0.461	0.698	7.69
1.0	Heterojunction	27.22	0.512	0.695	9.68
	Homojunction	26.88	0.487	0.72	9.42
10	Heterojunction	29.31	0.544	0.70	11.16
	Homojunction	28.69	0.494	0.744	10.545

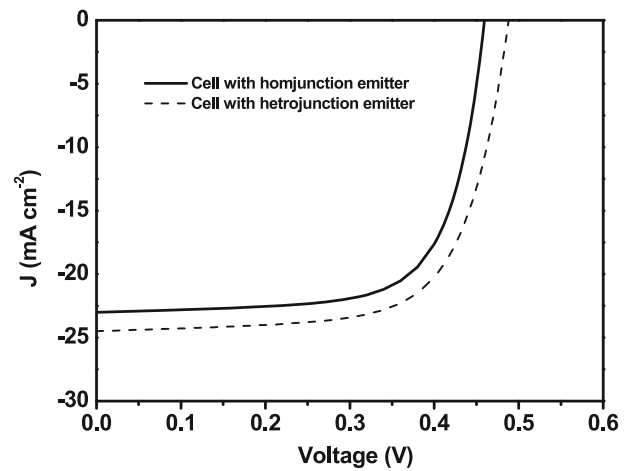


Fig. 4. The calculated $J - V$ characteristics of the homojunction and the heterojunction p^+-n-n^+ poly-Si solar cells with 0.1 μm grain size.

Figure 4. Table 2 shows the simulated results for the poly-Si solar cell with the homojunction and the heterojunction emitters, and with the poly-Si layers of 0.1, 1.0, and 10 μm grain sizes. The highest efficiency of 11.16% is obtained for the cell with 10 μm grain size. It is found that for all the three grain sizes studied, V_{oc} and J_{sc} are higher for the heterojunction cell as compared to the homojunction cell (Tab. 2). However, the FF of all the heterojunction cells is less than that of the homojunction cells. This is due to a large band gap difference between the a -Si emitter and the poly-Si absorber layers, which produces a large barrier in the vicinity of the interface and prevents the transportation of the photo excited carriers. Also, higher interface states at the interface of the a -Si emitter and the poly-Si absorber layers increases the recombination velocity and reduces the FF . In this study, we have taken into consideration the higher recombination velocity at the interface of the a -Si and the poly-Si. To minimize the interface effect, a thin μc -Si layer having a band gap intermediate between that of the a -Si and the poly-Si is considered at the interface of the a -Si and the poly-Si layer, and the results are shown in Section 3.3.

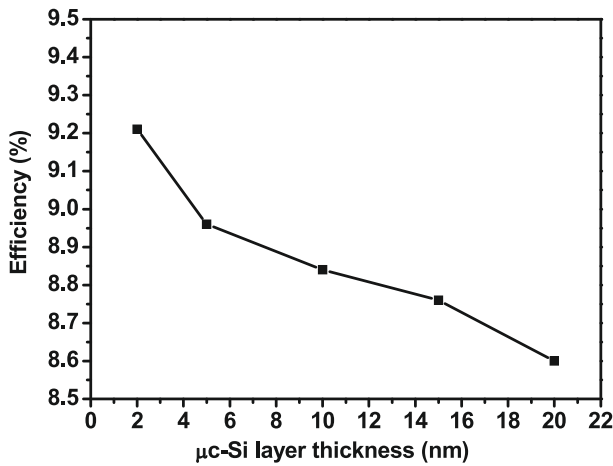


Fig. 5. The calculated efficiency versus $\mu\text{c-Si}$ layer thicknesses for the heterojunction $p^+ - n - n^+$ poly-Si cell with $0.1 \mu\text{m}$ grain size.

3.3 The poly-Si $p^+ - n - n^+$ heterojunction cell with a thin $\mu\text{c-Si}$ layer at the interface of $a\text{-Si}$ and poly-Si layers

The higher performance of the poly-Si $p^+ - n - n^+$ heterojunction cell with the $a\text{-Si}$ emitter is limited by the large number of interface states, dangling bonds and lattice mismatch between the $a\text{-Si}$ and the poly-Si. To further improve the performance of the cell, a thin $\mu\text{c-Si}$ layer is introduced between the $a\text{-Si}$ and the poly-Si layers for reducing the recombination of carriers at the interface. The $\mu\text{c-Si}$ layer, having band gap intermediate between that of the $a\text{-Si}$ and the poly-Si materials at the interface lowers the barrier produced by the direct contact of the materials having large band gap differences and also facilitates the transportation of the photoexcited carriers through the interface, resulting in a restraining of the recombination. Another advantage is seen in that the $\mu\text{c-Si}$ layer reduces the lattice mismatch between the poly-Si and the $a\text{-Si}$ layers. In order to illustrate the advantages of introducing the $\mu\text{c-Si}$ layer, simulations are carried out with the heterojunction emitter by introducing a thin $\mu\text{c-Si}$ layer at the interface of the $a\text{-Si}$ emitter and the poly-Si absorber layers, which is aimed at reducing the recombination of carriers. The results obtained are very much encouraging with better fill factor and higher efficiency.

Figure 5 shows the effect of the $\mu\text{c-Si}$ layer thickness on the performance of the cell. As the layer thickness increases, the efficiency slowly decreases and it is found that a thinner layer is needed for the optimum performance of the cell. For the 2 nm layer thickness, an efficiency of 9.21% is obtained which is 10% higher than the efficiency of the cell without this intermediate layer. The other photovoltaic parameters obtained are: $J_{sc} = 26.27 \text{ mA cm}^{-2}$, $V_{oc} = 0.487$, and $FF = 0.72$, for a grain size of $0.1 \mu\text{m}$. Figure 6 shows the $J - V$ characteristics of this cell and that of the cell without the $\mu\text{c-Si}$ layer (Fig. 4) for a comparison. An interesting point that is to be noticed is the increase in the FF of the cell with the $\mu\text{c-Si}$ layer from 0.684 to 0.72 with this modification, without any noticeable change in

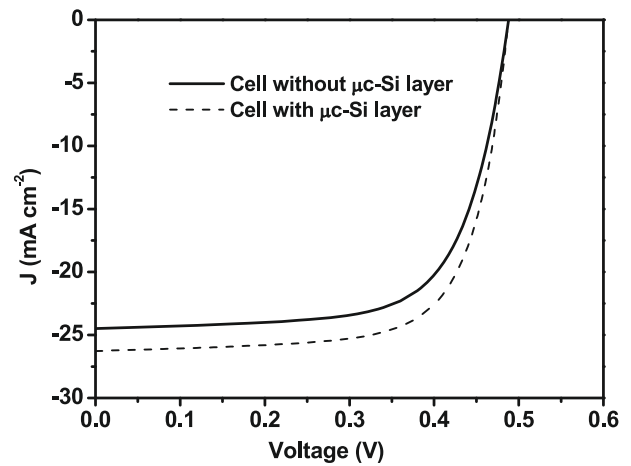


Fig. 6. The calculated $J - V$ characteristics of heterojunction $p^+ - n - n^+$ poly-Si solar cells with and without a thin $\mu\text{c-Si}$ layer and for $0.1 \mu\text{m}$ grain size.

Table 3. The simulated results obtained for the heterojunction $p^+ - n - n^+$ poly-Si cells with and without a $\mu\text{c-Si}$ thin layer for different grain sizes.

Grain size (μm)	Heterojunction cell	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF	η (%)
0.1	With $\mu\text{c-Si}$ layer	26.67	0.487	0.72	9.21
	Without $\mu\text{c-Si}$ layer	24.60	0.49	0.684	8.24
1.0	With $\mu\text{c-Si}$ layer	28.64	0.51	0.742	10.84
	Without $\mu\text{c-Si}$ layer	27.22	0.512	0.695	9.68
10	With $\mu\text{c-Si}$ layer	30.14	0.552	0.761	12.66
	Without $\mu\text{c-Si}$ layer	29.31	0.544	0.70	11.16

J_{sc} or V_{oc} . This indicated the reduced recombination effect of the interface between the $a\text{-Si}$ and the poly-Si layers. Table 3 shows the results obtained for the poly-Si $p^+ - n - n^+$ heterojunction cell with the $a\text{-Si}$ emitter with and without the $\mu\text{c-Si}$ thin layer, for grain sizes of $0.1 \mu\text{m}$, $1 \mu\text{m}$, and $10 \mu\text{m}$.

In all these cases, an increase in the performance of the cell is evident, which is due to the improved FF . The highest efficiency of 12.66% is obtained for the cell with $10 \mu\text{m}$ grain size. The other photovoltaic parameters obtained for this cell are: $J_{sc} = 30.14 \text{ mA cm}^{-2}$, $V_{oc} = 0.552 \text{ V}$, $FF = 0.761$. Thus, larger grain size and well passivated grain boundary with reduced recombination at the interface of the $a\text{-Si}$ emitter and the poly-Si absorber layers resulted in higher efficiency poly-Si $p^+ - n - n^+$ thin film solar cell.

4 Conclusion

In this study, we analyzed the performance of $p^+ - n - n^+$ homojunction cell with well passivated, partially passivated and least passivated grain boundaries and the results revealed that well passivation of the defects at the grain boundary is the key for achieving higher efficiency poly-Si solar cells. Higher V_{oc} values are possible for the poly-Si thin film solar cell with small grain sizes when a thin a -Si emitter layer is used. Also, by the careful design of the cell structure with interface layers, it is possible to obtain higher efficiencies for the poly-Si solar cells.

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