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RESEARCH

Investigation of the impact of different ARC layers using PC1D simulation: application to crystalline silicon solar cells

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Abstract

In this work, the impact of six different anti-reflection coating (ARC) layers has been investigated using PC1D simulation software. Simulation shows that the range of 500–700 nm would be suitable for designing an ARC. Designing a single-layer silicon nitride (Si_3N_4) ARC for 600 nm wavelength and with a thickness of 74.257 nm, a silicon solar cell with 20.35% efficiency has been simulated. Very closely followed by a 20.34% efficient silicon solar cell with 74.87 nm thick zinc oxide (ZnO) ARC layer. Significant increase in efficiency has been observed by applying ARC in respect to not applying any kind of ARC. After efficient solar cell modeling, optimum efficiency of 20.67% is being achieved by using SiO_2 surface passivation and Si_3N_4 ARC layer. The effects on voltage, current, photovoltaic efficiency, reflectivity and external quantum efficiency due to ARCs are also represented in this work.

Keywords Silicon solar cell · Anti-reflection coating (ARC) · Surface passivation · External quantum efficiency (EQE)

Introduction

One of the important issues of modern photovoltaic science is the optical losses in solar cell. In general, the optical losses account for about 7% efficiency loss in crystalline silicon solar cells [1]. So, the reduction in optical loss can have a huge positive impact on the conversion efficiency of silicon solar cells [2]. To reduce the optical loss, anti-reflection coating (ARC) plays a pivotal role in reducing reflection thus increasing the conversion efficiency of solar cells [3]. Anti-reflection coating reduces reflection by using the concept of phase changes in light and the dependence of the reflectivity on refractive index [4]. Since the fabrication of solar cell, many researchers used different ARCs, and still searching for a suitable ARC which can be used to improve the efficiency of solar cell [5, 6].

In the experimental study of ARC, Hocine et al. used TiO_2 on crystalline silicon solar cell and found an increased efficiency of 14.26%, whereas without TiO_2 the efficiency is limited to 11.24% [7]. Similarly Swatowska et al. [8] found an efficiency of 9.84% for a crystalline silicon solar cell without any ARC, and efficiencies of 14% and 14.25% are obtained using TiO_2 and Si_3N_4, respectively. In another study, Gee et al. [9] fabricated 15.55% and 16.03% efficient crystalline silicon solar using TiO_2 and ZnO, respectively. It thus turns out that ZnO would be an appropriate choice among those different ARCs. However, in all cases the wafer size, fabrication process and the condition were different. For instance, Hocine et al. used a 5×5 cm^2 wafer and Swatowska et al. considered 10×10 cm^2 wafer. Thus, comparing different works is really a challenge and result cannot be always conclusive. Moreover, designing ARC is a difficult task because of having so many options in parameters and materials. Little change in any aspect of ARC fabrication is challenging and costly. Therefore, researchers are now giving importance in doing simulation before actual fabrication. This is because through simulation, parameters can be defined and changed, similar environment can be considered in all cases, and selection of materials can be done quite easily. Moreover, theoretical investigations can be observed and studied in depth [10].

In the simulation study of ARC, Abdullah et al. [6] used Silvaco ATLAS to simulate silicon solar cell and obtained

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4.72% efficient solar cell using 5 nm SiO_2 coating. Also, Lennie et al. used the similar tool and using double-layer SiO_2/Si_3N_4 anti-reflection coating the simulated solar cell exhibited an efficiency of 4.56% [11]. In Ref. [12–15], there were reports on simulation work using PC1D. Although same software was used in all their works, however, different ARCs and materials have been used by them. For instance, Moradi et al. [13] found 10.78%, 11.7% and 11.89% efficiency using TiO_2, ZnO and Si_3N_4 single-layer ARC, respectively, upon silicon solar cell. Also, the efficiencies of 13.37% and 13.59% are shown using ZnO/TiO_2 and SiO_2/TiO_2 double-layer ARC, respectively. Using ZnO and ZnS ARC, Naser et al. simulated 18% and 19% efficient silicon solar cell with, respectively [15]. Thosar et al. simulated GaAs solar cell and showed that optimum short-circuit current can be found using ZnO and MnO ARC with 65 nm and 80 nm thicknesses, respectively [14]. Daniel N. Wright et al. reported 6.7% efficient solar cell with Si_3N_4 and SiO_2 ARC upon crystalline silicon wafers [12]. Yahia et al. [16] performed simulation using MATLAB to see the effects of ARC on silicon substrate. From these researches, it indicates that MATLAB, PC1D, Silvaco ATLAS are used to simulate ARC of solar cell [11, 12, 16]. However, MATLAB software does not provide rigorous options of solar cell. On the other hand, PC1D is the most commercially available software used by many companies and universities [17]. Also, depending upon availability PC1D version 5.9 has been used to simulate solar cell with different types of ARC layers.

The vast majority of ARC simulation studies indicate generally two or three single-layer ARC upon silicon solar cell with 3–13% efficiency [6, 12–16]. However, no reports were found showing the suitable wavelength for designing ARC and utilizing the concept of surface passivation upon ARC. Thus, to overcome all these issues and to perform a systematic study the main goal of this work is to simulate different types of ARCs and find out the suitable ARC for crystalline silicon solar cell. In this research, the impact without ARC and with six types of ARCs such as titanium dioxide (TiO_2), zinc oxide (ZnO), zinc sulfide (ZnS), silicon dioxide (SiO_2), silicon nitride (Si_3N_4) and silicon carbide (SiC) has been investigated separately for crystalline silicon solar cell. Furthermore, simulation ranging from 250 to 1200 nm wavelength has been conducted to find out the most suitable wavelength required for designing ARC in solar cell. The reason for using these wavelengths is that the solar spectrum covers this range. Also, these wavelengths can be easily experimentally generated by UV-VIS-NIR spectrophotometer. Surface passivation upon ARC has been applied, and its impact has been investigated. The ARC simulation also gives insight into its effects on efficiency of solar cell. Moreover, the reflectivity for the wavelength range of 250–1250 nm of all the ARCs and external quantum efficiency has also been discussed in this paper.

Simulation

Simulation without ARC

To simulate the solar cell without ARC (Fig. 1a), a P-type silicon wafer with an area of 10×10 cm^2 and thickness of 300 µm has been chosen. Afterward, the doping concentration of P-type has been selected to 1×10^{17} cm^{-3}. Then, the subsequent N-type silicon layer thickness and doping concentration has been adjusted to 2 µm and 1×10^{18} cm^{-3}, respectively [18]. In both P-type and N-type layers, a uniform doping profile has been assumed. Typically, the diffusion length of mono-crystalline silicon solar cell is 100–300 µm [19].

The diffusion length has to be less than the P-type wafer thickness of 300 µm. Note that the minimum minority carrier life time allows to limit the diffusion length less than 130 µm [20]. Thus, for realistic approach the diffusion length of 200 µm is considered here. To enhance the absorption,

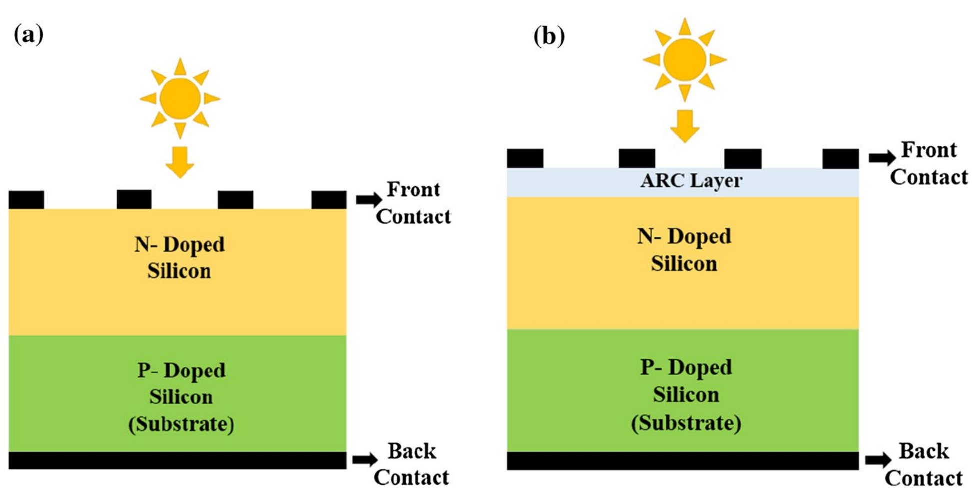

Fig. 1 Simplified solar cell schematic without ARC (**a**) and with ARC (**b**)

experimentally obtained textured wafer data were considered and inputted in this simulation. Both sides texturing option was enabled, and pyramid height of 1 µm with equal angles of 54.74° was considered for initial simulation. This is because in Ref. [18], the pyramid height of textured wafer height lies in the range of 1–3.5 µm, obtained following the etching solution of 0.763 wt% KOH–4 wt% IPA. Finally, to emulate the sun, AM (air mass) 1.5 G and 100 number of time steps have been selected.

Simulation with different ARCs

To introduce ARC layer, the front surface optically coated option has been selected in the simulation. Then, the refractive index and thickness have been varied according to different ARCs. A simplified solar cell schematic with ARC is shown in Fig. 1b. Now, in order to design and understand the behavior of the ARC layer, the following equations [21–24] are necessary.

$$\hat{n}(\lambda) = n(\lambda) + i\kappa(\lambda) \tag{1}$$

where $\hat{n}(\lambda)$ is the complex refractive index. In complex refractive index, there is real part called real refractive index $n(\lambda)$, and an imaginary part called extinction coefficient $\kappa(\lambda)$ and both are functions of wavelength. The absorption coefficient $\alpha(\lambda)$ is related to the extinction coefficient k by the following relation

$$\alpha(\lambda) = \frac{4\pi}{\lambda}\kappa(\lambda) \tag{2}$$

It is clear that from Eq. 2 that the photons (or radiation) that are absorbed depend on the wavelength, thickness and nature of the medium [24].

Now the refractive index of ARC is $\eta_{ARC} = \sqrt{\eta_{air} \times \eta_{arc}(\lambda_0)}$ (3)

and the thickness of ARC is $d = \frac{\lambda_0}{4 \times \eta_{ARC}}$ (4)

Here, η_{air} is the refractive index of air and η_{arc} is the refractive index of an anti-reflection coating for a specific wavelength (λ_0). Closer inspection of Eq. 3 shows that refractive index of ARC depends on refractive index of air as well as wavelength-dependent refractive index of a particular anti-reflection coating. Nevertheless, the value of right-hand side of Eq. 3 was not inputted in Eq. 3 or in the simulation. From Ref. [25–30], experimentally obtained η_{ARC} values for different ARCs ranging from 250–1200 nm have been directly inputted in Eq. 4 and then in the simulation. Inputting wavelength (λ_0) and corresponding η_{ARC} value determines the associated optimum thickness values for each ARC. All the wavelengths, thicknesses, refractive indexes, V_{OC}, I_{SC} and efficiencies are tabulated in Table 1. Then, with the optimum thickness and its corresponding η_{ARC} values, performances of different ARC layers have been studied through reflectance.

It is well known that high surface recombination rate reduces short-circuit current and thus the efficiency of solar cells. The surface recombination of photo-excited electron–hole pair takes place because of the dangling bonds at the top of surface. By reducing the number of dangling bonds, surface recombination can be lowered. Generally, a technique called thermal oxidation is used to reduce the surface recombination. In thermal oxidation technique, a "passivating" layer is grown thermally. The surface-passivating layer is fabricated with silicon oxide (SiO_2) which is used to passivate the surface. By applying only O_2 gas, SiO_2 layer can be grown upon Si_3N_4 layer [31]. As Si_3N_4 ARC shows the highest efficiency (discussed in"Effects of ARC" section), in this work, surface-passivated layer that is a simulation of SiO_2 layer upon Si_3N_4 ARC layer has been done.

In the simulation to see the external quantum efficiency and reflectivity of each ARC layer, excitation option has been modified from "one sun" to "SCAN-QE" (scan quantum efficiency). Furthermore, for better analysis, the number of time steps has been increased to 200 and the monochromatic wavelength spectrum range has been selected from 250 to 1250 nm. Then, the simulation data of external quantum efficiency and reflectivity have been obtained and analyzed for every single ARC.

Results and discussion

Effects of ARC

By analyzing the data of different ARCs in Table 1, it is seen that changing wavelength along with its thickness also changes the V_{OC}, I_{SC} and the efficiency of the solar cell. As absorption coefficient, refractive index, excitation coefficient are wavelength-dependent and cannot be changed easily, only thickness of the film can be optimized to get optimum absorption thus getting maximum V_{OC}, I_{SC} and efficiency. In the case of SiC, the table reveals that optimum thickness of SiC ARC is 36.159 nm. For that thickness, maximum of 16.06% efficiency has been achieved. Maximum V_{OC} and I_{SC} value of 0.6779 V and 2.807 A is being achieved at the best efficiency. The optimum thickness and efficiency with TiO_2, ZnO, ZnS, SiO_2 and Si_3N_4 ARC for solar cell are 62.396, 78.411, 63.479, 101.351 and 74.257 nm and 19.73%, 20.34%, 19.83%, 18.99% and 20.35%, respectively. The reason for such efficiency increase is the reduction in light reflection [32]. As the thickness increases, V_{OC}, I_{SC} and efficiency also increases up to the point where reflection is the lowest (Fig. 2). Then, V_{OC}, I_{SC} and efficiency of

Table 1 Data of different ARCs

λ	SiC ARC					TiO_2 ARC					ZnO ARC				
λ	Refractive index [25]	Thickness (nm)	I_{SC} (A)	V_{OC} (V)	η	Refractive index [26]	Thickness (nm)	I_{SC} (A)	V_{OC} (V)	η	Refractive index [27]	Thickness (nm)	I_{SC} (A)	V_{OC} (V)	η
250	3.25	19.231	2.655	0.6765	15.14%	2.46	25.407	2.789	0.6777	15.95%	2.388	26.173	2.797	0.6778	16.00%
300	3.528	21.259	2.649	0.6765	15.10%	3.326	22.55	2.712	0.677	15.49%	2.404	31.198	2.937	0.6791	16.84%
400	3.519	28.417	2.75	0.6774	15.72%	2.68	37.213	3.313	0.6808	18.00%	2.114	47.304	3.269	0.682	18.82%
500	3.457	36.159	2.807	0.6779	16.06%	2.48	50.403	3.358	0.6828	19.36%	1.968	63.516	3.467	0.6838	20.01%
600	3.406	44.04	2.802	0.6778	16.03%	2.404	62.396	3.42	0.6834	19.73%	1.913	78.411	3.523	0.6843	20.34%
700	3.358	52.114	2.773	0.6776	15.86%	2.364	74.027	3.377	0.683	19.47%	1.883	92.937	3.473	0.6839	20.04%
800	3.315	60.332	2.736	0.6772	15.63%	2.341	85.434	3.247	0.6821	18.85%	1.864	107.296	3.359	0.6829	19.36%
900	3.285	68.493	2.702	0.6769	15.44%	2.325	96.774	3.156	0.681	18.14%	1.851	121.556	3.226	0.6817	18.56%
1000	3.247	76.994	2.686	0.6768	15.34%	2.313	108.085	3.06	0.6802	17.57%	1.841	135.8	3.109	0.6806	17.86%
1100	3.228	85.192	2.708	0.677	15.47%	2.305	119.306	2.997	0.6796	17.19%	1.833	150.027	3.023	0.6798	17.35%
1200	3.2	93.75	2.719	0.6771	15.54%	2.298	130.548	2.953	0.6792	16.93%	1.826	164.294	2.963	0.6793	16.99%
	ZnS-ARC					SiO_2-ARC					Si_3N_4-ARC				
λ	Refractive index [28]	Thickness (nm)	I_{SC} (A)	V_{OC} (V)	η (%)	Refractive index [29]	Thickness (nm)	I_{SC} (A)	V_{OC} (V)	η (%)	Refractive index [30]	Thickness (nm)	I_{SC} (A)	V_{OC} (V)	η (%)
250	2.6	24.038	2.771	0.6776	15.85	1.52	41.12	2.757	0.6774	15.76	2.289	27.304	2.805	0.6779	16.05
300	2.57	29.183	2.909	0.6788	16.67	1.51	49.67	2.87	0.6785	16.44	2.167	34.61	2.962	0.6793	16.99
400	2.56	39.063	3.176	0.6812	18.26	1.5	66.67	3.097	0.6805	17.79	2.07	48.31	3.271	0.6821	18.83
500	2.421	51.632	3.382	0.6831	19.50	1.482	84.35	3.242	0.6818	18.66	2.03	61.576	3.468	0.6838	20.01
600	2.363	63.479	3.437	0.6836	19.83	1.48	101.351	3.297	0.6823	18.99	2.02	74.257	3.525	0.6843	20.35
700	2.332	75.043	3.39	0.6831	19.55	1.474	118.72	3.263	0.682	18.79	2.003	87.369	3.475	0.6839	20.05
800	2.324	86.059	3.28	0.6821	18.89	1.473	135.78	3.18	0.6813	18.29	1.996	100.2	3.361	0.6829	19.37
900	2.31	97.403	3.161	0.6811	18.17	1.472	152.85	3.078	0.6803	17.68	1.991	113	3.227	0.6817	18.57
1000	2.301	107.648	3.071	0.6803	17.63	1.471	169.95	2.984	0.6795	17.11	1.987	125.82	3.113	0.6806	17.88
1100	2.296	119.774	2.999	0.6796	17.20	1.47	187.07	2.911	0.6788	16.68	1.985	138.54	3.031	0.6799	17.40
1200	2.29	131.004	2.954	0.6792	16.94	1.469	204.22	2.86	0.6784	16.37	1.983	151.28	2.974	0.6794	17.06

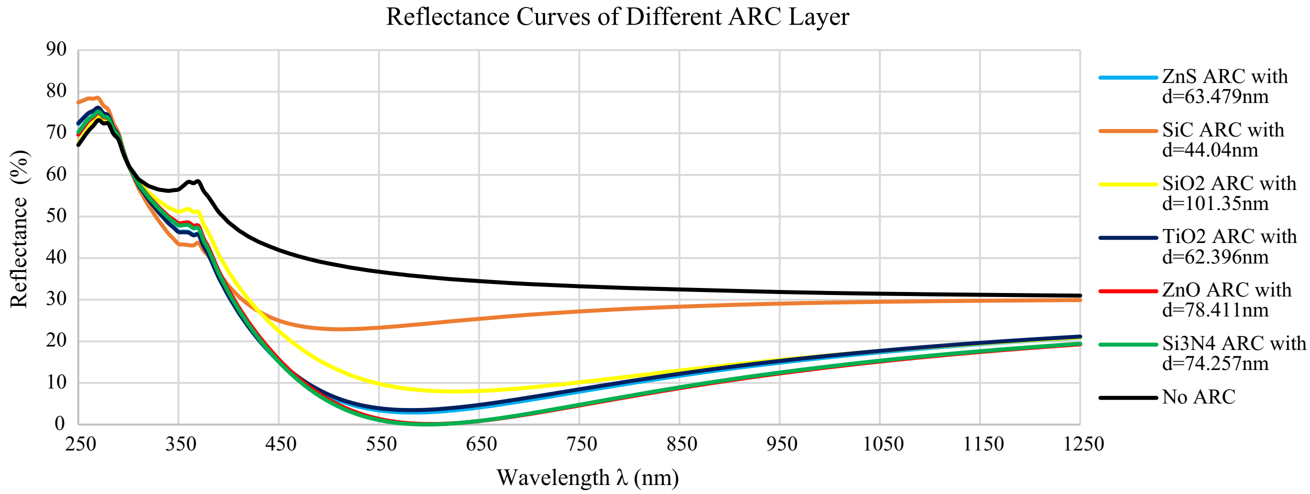

Fig. 2 Reflectance curves of different ARC layers designed for 600 nm wavelength with associated thickness

solar cell decrease as reflection increases. So, the optimization of thickness is required to get the lowest reflectance and to obtain the best V_{OC}, I_{SC} and efficiency. Surprisingly, except SiC ARC, for all other ARCs the highest efficiency is achieved at a wavelength of 600 nm. This can be seen in Fig. 2. It is seen that at a wavelength of 600 nm, for SiC, TiO_2, ZnO, ZnS, SiO_2 and Si_3N_4 ARC the reflectance is 24.31%, 3.59%, 0.136%, 2.98%, 8.14% and 0.032%, respectively. Overall, the lowest reflectance curve (green) is for Si_3N_4 ARC closely followed by the Red reflectance curve of ZnO ARC. The Black curve signifies the general representation of a solar cell reflectance curve without any ARC. As can be seen from the Black curve, there are two peaks and afterward the curve decreases and then it becomes somewhat constant. But for all the reflectance curves with ARC, after two peaks the curves decrease rapidly up to a point then again increases. It is in good agreement of the results shown in Table 1, as the similar behavior is observed in the case of efficiency. The summary of Table 1 is for 74.257 nm thickness Si_3N_4 ARC for solar cell shows the finest result with 20.35% efficiency. It is fascinating that without any ARC, the efficiency of solar cell is 14.02%. So, after applying ARC significant increase in efficiency is observed. Now to find out the explanation of decrease in reflectance up to a certain point and then an increase in the reflectance curve in Fig. 2, the wavelength and associated thickness of Si_3N_4 ARC have been varied and the result is tabulated in Table 2. The reason for choosing only Si_3N_4 ARC is that it has the best solar cell efficiency mentioned earlier (Table 1). It is seen form Table 2 that if Si_3N_4 ARC is designed for 500 nm wavelength and with 61.576 nm thickness then the reflectance is lowest at 500 nm. At 500 nm, Si_3N_4 ARCs reflectance is 0.045%, whereas at 600 and 700 nm the reflectance is 3.677% and 8.957%, respectively. Similarly, if Si_3N_4 ARC is designed for 600 nm wavelengths and with 74.257 nm thickness then reflectance at 500, 600 and 700 nm is 5.537%, 0.0317% and 2.644%, respectively. It is interesting that the particular wavelength and associated thickness for which the ARC is designed show the lowest reflectance. So, in all the ARC reflectance curves in Fig. 2, the reflectance decreases after the two peaks up to 600 nm wavelength and associated thickness for which the ARC has been designed. It is suffice to say after observing all the reflectance curves in Fig. 2 that when the reflection of light from the surface is reduced, the efficiency of solar cell is increased.

Effects of surface passivation

As stated earlier, solar cell with Si_3N_4 ARC has the best efficiency of 20.35%, and surface passivation (SiO_2 layer) has been applied only upon this layer. Table 1 indicates that the optimum thickness of SiO_2 and Si_3N_4 layer is 101.351 nm

Table 2 Data of Si_3N_4 ARC

ARC (Si_3N_4)	Reflectance (%) at 500 nm wavelength	Reflectance (%) at 600 nm wavelength	Reflectance (%) at 700 nm wavelength	Efficiency (%)
$\lambda = 500$ nm, $d = 61.576$ nm	0.045	3.677	8.957	20.01
$\lambda = 600$ nm, $d = 74.257$ nm	5.537	0.0317	2.644	20.35
$\lambda = 700$ nm, $d = 87.369$ nm	17.716	3.462	0.094	20.05

and 74.257 nm, respectively; thus, these two thicknesses were used in the simulation for surface passivation first and after completion of simulation the data were tabulated in Table 3. It indicates that maximum of 20.42% efficiency can be achieved by applying 101.351-nm-thick SiO_2 layer upon 74.257-nm-thick Si_3N_4 layer. However, through optimization one can reduce the layer thickness as can be seen from Table 3 that optimum efficiency of 20.67% is being achieved with 57-nm-thick SiO_2 layer upon 58-nm-thick Si_3N_4 ARC. This is because the SiO_2 surface-passivated layer upon Si_3N_4 ARC behaves like double-layer ARC and for that refractive index, thickness and reflectivity of the ARC layer follow a complex equation. For details, see Ref. [33]. It also signifies that optimum surface passivation reduces both SiO_2 and Si_3N_4 layer thickness; thus, in actual fabrication process overall fabrication cost may be reduced. The reflectivity curve in Fig. 3 also confirms the complex behavior of surface-passivated layer. Unlike the Si_3N_4 ARC (green curve), there is an increase in reflectance around 600 nm regions for surface-passivated blue curve, whereas the surface-passivated Red reflectance curve overall has lower reflectance in the 250–1250 nm wavelength region than other reflectance curves. The fact is that the efficiency is increased due to the reduction in reflection light and occurred because of surface passivation process.

Result of external quantum efficiency (EQE) is shown in Fig. 4. Upon inspection of Fig. 4, it can be concluded that after utilization of ARC, EQE has increased significantly. This increase is due to the reduction in reflection for applying ARC. Although from 425 to 640 nm the EQE of Si_3N_4 ARC (Black) curve is slightly greater than EQE of Si_3N_4 ARC (Red) curve, from 640 nm and overall the EQE is showing the best result for the surface-passivated curve (Red). It is adequate to say, surface passivation increases the overall EQE of solar cell by reducing the number of dangling bonds thus reducing the recombination effects [34, 35].

Conclusion

The effect of different single-layer ARCs has been investigated using PC1D simulation software. It is seen in the literature that Gee et al. fabricated 15.55% and 16.03% efficient solar cell with TiO_2 and ZnO ARC, respectively. However, in the simulation it is seen that 15.49% and 16.00% efficient solar cell has been obtained with TiO_2 and ZnO ARC, respectively. To obtain these efficiencies, thickness of with TiO_2 and ZnO ARC was considered 22.55 nm and 26.173 nm, respectively. Efficiency can be further increased with TiO_2 and ZnO ARC in the simulation by optimizing thickness and other parameters. The same thing can be said for other ARCs also. So it can be said that there is little difference in the result obtained from simulation than experimental results. Simulation shows that the range of 500–700 nm would be suitable for designing an ARC. Among TiO_2, ZnO, ZnS, SiO_2, Si_3N_4 and SiC ARC, Si_3N_4 ARC exhibits the best performance with an efficiency of 20.35% for crystalline silicon solar cell. Then, ZnO ARC is indicating the second best performance with an efficiency of 20.34%. However, without any ARC the efficiency of solar

Table 3 Associated parameters of solar cell with surface-passivated ARCs

Surface passivation conditions	Short-circuit current (I_{SC})	Open-circuit voltage (V_{OC})	Max power (W)	Fill factor (FF)	Efficiency (%)
101.351 nm SiO_2/74.257 nm Si_3N_4 ARC	3.535 A	0.6844 V	2.042	0.8440	20.42
57 nm SiO_2/58 nm Si_3N_4 ARC	3.576 A	0.6848 V	2.067	0.8441	20.67

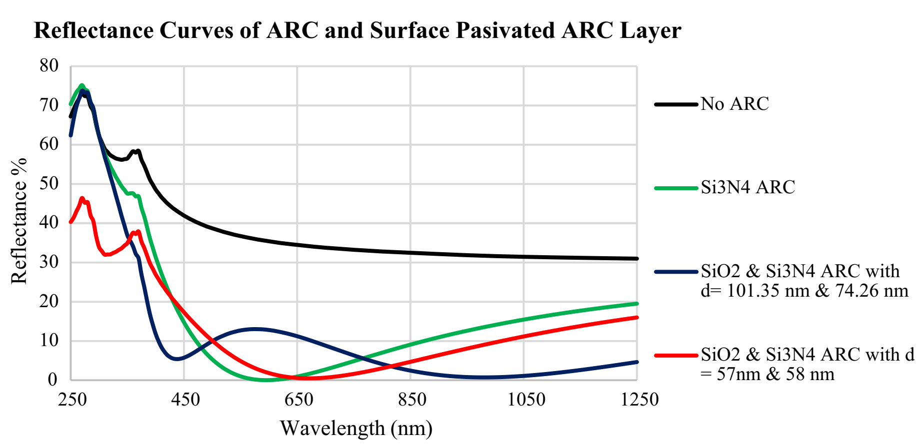

Fig. 3 Reflectance curves of ARC and surface-passivated ARC layer

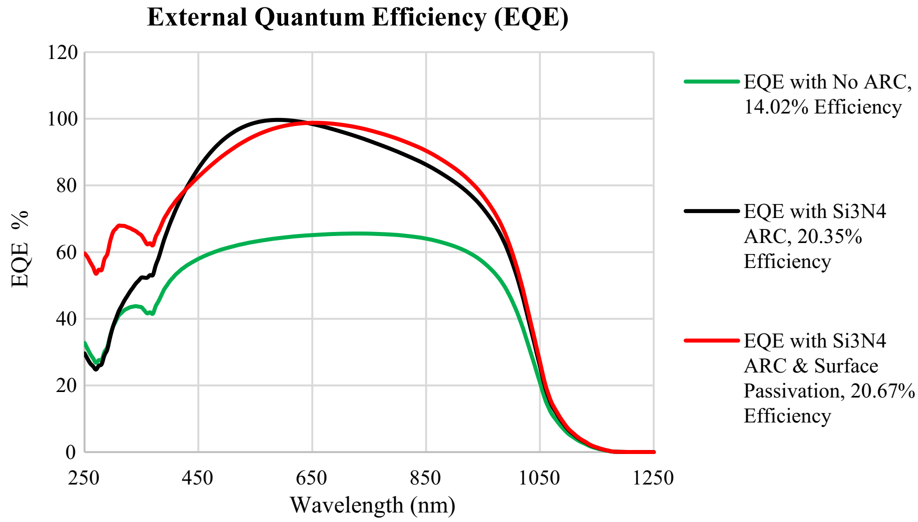

Fig. 4 External quantum efficiency curves

cell is 14.02%. So, after applying ARC significant increase in efficiency is observed. The reason for such efficiency increase is due to the reduction in reflection. So applying anti-reflection coating would be a good choice to enhance the efficiency. Also, SiO_2 surface passivation treatment on Si_3N_4 ARC layer was performed and 20.67% efficient solar cell is being achieved. Increase in EQE and decrease in reflectance also confirm that surface-passivated layer upon ARC increases the efficiency of solar cell.

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