

Fabrication of Single Layer SiO₂ and Si₃N₄ as Antireflection Coating on Silicon Solar Cell Using Silvaco Software

¹A. Lennie, ¹H. Abdullah, ²S. Shaari and ³K.Sopian

¹Department of Electrical, Electronics and Systems Engineering,
Faculty of Engineering and Built Environment, University Kebangsaan Malaysia,
43600 Bangi Selangor, Malaysia

²Laboratory of Photonics Technology, Institute of Microengineering and Nanoelectronics,
University Kebangsaan Malaysia, 43600 Bangi Selangor, Malaysia

³Solar Energy Research Institute, University Kebangsaan Malaysia, 43600 Bangi Selangor, Malaysia

Abstract: The main objectives was to investigate and enhance the short circuit current density, J_{sc} and also to improve the efficiency of silicon solar cell by fabricating a layer of silicon dioxide (SiO₂) and silicon nitride (Si₃N₄) coatings on silicon solar cell. This fabrication carried out on high temperature during annealing process from 800-1050°C and variable thickness of antireflection coating (ARC) layer from 50-90 nm thick. The photovoltaic properties of Si₃N₄ layer have been compared with SiO₂ layer to determine which material is suitable in fabricating single layer ARC. Solar cell simulation could be useful for time saving and cost consumption. **Problem statement:** The Silvaco software is not widely used in designing the 2D solar cell devices because there are lots of 1D, 2D and 3D-simulation beside Silvaco software such as MicroTec, SCAPS-1D. **Approach:** The silicon dioxide (SiO₂) and silicon nitride (Si₃N₄) coating have been modeled and fabricated on silicon solar cell by using Silvaco software packaging. **Results:** For SiO₂ results, the FF value is approximately 0.758 and η maximum 9.43%. In annealing process, the temperature becomes higher resulted increasing of pn junction depth. However, not to V_{oc} and J_{sc} values, both parameters were slowly decreased when temperature increased. Meanwhile, when the thickness of SiO₂ layer is increased, the parameters of pn junction depth, J_{sc} , V_{oc} , FF and η were decreased slowly. As for Si₃N₄ result, the calculated FF approximately 0.758 and η maximum is 9.57%. During annealing process, the temperature increasing constantly follows the increasing of pn junction depth and J_{sc} , meanwhile the V_{oc} is decreased slowly. In variable Si₃N₄ thickness simulation, the output parameters of pn junction depth, J_{sc} , V_{oc} , FF and η were decreased when the thickness increased 10 nm each simulation. **Conclusion:** The optimum temperature during annealing process for SiO₂ is 950°C, while for Si₃N₄ is 1050°C. For the thickness analysis, the optimum ARC thickness for SiO₂ and Si₃N₄ layer is 50 nm both.

Key words: Silicon solar cell, SiO₂, Si₃N₄, efficiency, Silvaco

INTRODUCTION

Traditional fuel energy resources are limited and generate harmful waste products in the atmosphere. Hence, alternative eco-friendly energy sources are receiving increasing attention. Of all substitute energy sources, solar power is most attractive because of its abundance and the consistency of sunlight^[1]. In 1950s, Chapin *et al.*^[2] at Bell laboratories developed the first crystalline silicon solar cell with a solar-energy conversion efficiency of 6%. However, the relatively

high cost of manufacturing these silicon cells has prevented them from extensive use. Moreover, another disadvantage of silicon cells is the use of toxic chemicals during manufacturing. Accordingly, the development of low-cost organic solar cells is urgent.

High quality Anti-Reflective Coatings (ARC) have become a vital feature of high-efficiency silicon solar cells^[3]. Several authors have conducted extensive studies in past few years to investigate the effects of various ARC on high efficiency monocrystalline and polycrystalline solar cells^[4]. Several materials having

Corresponding Author: H. Abdullah, Department of Electrical, Electronics and Systems Engineering,
Faculty of Engineering and Built Environment, University Kebangsaan Malaysia,
43600 Bangi Selangor, Malaysia

the appropriate refractive index have been proposed and used for single or double layer ARC, such as TiO_2 ($n = 2.2$), MgF_2 ($n = 1.35$), ZnS ($n = 2.3$), CVD SiN ($n = 1.6-2.4$) and SiO_2 ($n = 1.46$). The thickness and refractive index play role in photoelectrical conversion by reducing the reflectivity losses. The refractive index of stoichiometric LPCVD Si_3N_4 is close to the calculated value of 2.3 for the top layer.

Silvaco TCAD offers complete and well-integrated simulation software for all aspects of solar cell technology. TCAD modules required for solar cell simulation include: S-Pisces, blaze, Luminous, TFT, Device3D, Luminous3D and TFT3D^[5]. S-Pisces is an advanced 2D device simulator for silicon based technologies that incorporates both drift-diffusion and energy balance transport equations. Large selections of physical models are available for solar cell simulation, which includes surface/bulk mobility, recombination, impact ionization and tunneling models. Blaze simulates 2D solar cell devices fabricated using advanced materials. It includes a library of binary, ternary and quaternary semiconductors. Blaze has built-in models for simulating state-of-the-art multi-junction solar cell devices. Luminous and Luminous3D are advanced 2D and 3D simulator specially designed to model light absorption and photogeneration in non-planar solar cell devices. Exact solutions for general optical sources are obtained using geometric ray tracing. This feature enables Luminous and Luminous3D to account for arbitrary topologies, internal and external reflections and refractions, polarization dependencies and dispersion. Luminous and Luminous3D also allows optical transfer matrix method analysis for coherence effects in layered devices. The beam propagation method may be used to simulate coherence effects and diffraction.

The purpose of this work is to investigate and enhance the short circuit current density, J_{sc} and also to improve the efficiency of silicon solar cell by fabricating single layer of SiO_2 and Si_3N_4 coatings on silicon solar cell using Silvaco TCAD software.

MATERIALS AND METHODS

The solar cell that has been chosen for test is made in usual method in VLSI. An orientation of silicon wafer is $\langle 100 \rangle$ with $50 \mu\text{m}$ thickness and boron concentration of $1 \times 10^{14} \text{ atom cm}^{-2}$ was chosen to create p-type silicon substrate. The p-n junction was developed by phosphorus implantation with $1 \times 10^{16} \text{ atom cm}^{-2}$ and energy is 30 eV. The diffuse time 60 min and temperature is variable parameter. The deposition of ARC also considered as variable parameter. The

ATHENA framework is used to design the 2D solar cell structure with area $50 \times 10 \mu\text{m}^2$. Then the voltage was applied on device by using ATLAS framework to compute open circuit voltage, V_{oc} and short circuit current density, J_{sc} . In this simulation, the incident light has been fixed to 90° angle. The 90° incident light was applied on the top of silicon solar cell to trace the reflectance in silicon wafer (Fig. 1 and 2). In first simulation, the variable temperature that has been decided to analyze is 800, 850, 900, 950, 1000 and 1050°C . Then the second simulation, the variable thickness for this analysis is 50-90 nm with interval 10 nm thick. Table 1 show the details of input data were used in modeling solar cell structure for both analyses.

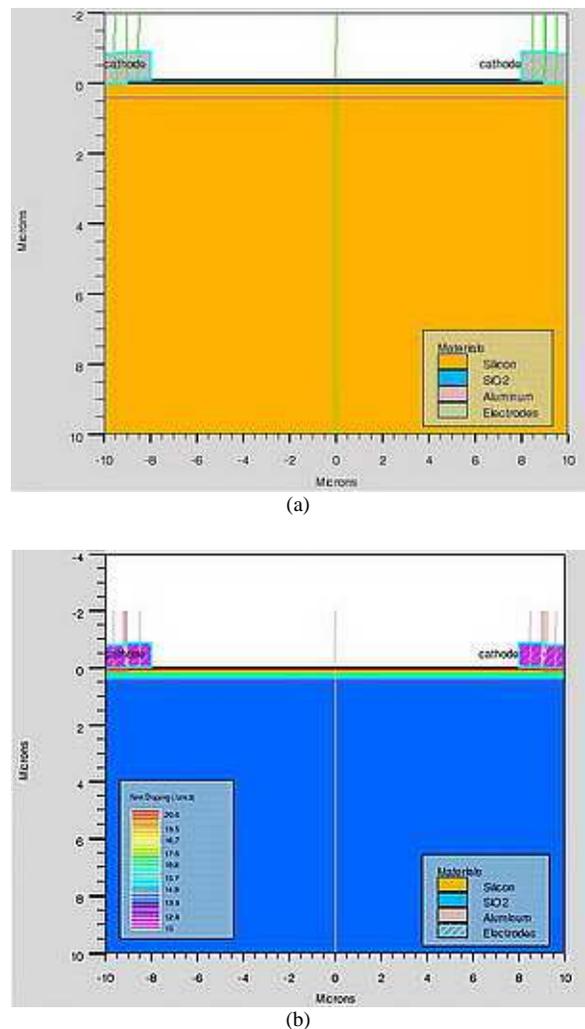


Fig. 1: The cross-section of $10 \times 10 \mu\text{m}^2$ solar cell structure with SiO_2 single layer coating; (a) basic color region. (b) net doping color region

Table 1: Input data were used in modeling solar cell structure for SiO₂ and Si₃N₄ simulation

Parameter	First simulation	Second simulation
Orientation	100	100
Device area (μm ²)	50 × 10	50 × 10
Phosphorus doping (atom m ⁻²)	1 × 10 ¹⁶	1 × 10 ¹⁶
Energy (eV)	30	30
Diffuse time (min)	60	60
Diffuse temperature (°C)	800, 850, 900, 950, 1000, 1050	950
ARC thickness (nm)	50	50, 60, 70, 80, 90
Incident light beam (°)	90	90

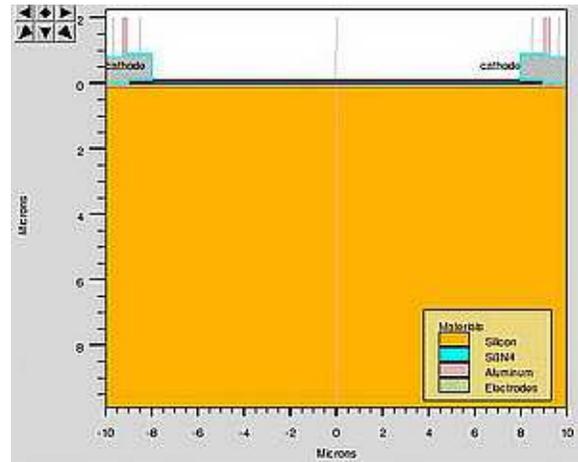
RESULTS

The solar cell structure has been modeled by using Silvaco TCAD tools. The variable temperature that has been simulated in first simulation is 800, 850, 900, 950, 1000 and 1050°C. Meanwhile the variable thickness that has been fabricated in second simulation is 50, 60, 70, 80 and 90 nm. After all simulations have been done running, the Athena framework will display the 2D device structure. Figure 1 and 2 illustrated cross-section of 10×10 μm² solar cell structure when heating in 950°C on 50 nm thick of SiO₂ and Si₃N₄ single layer, respectively, in first simulation. In this study, the simulation only concentrated on normal incident light beam for both ARC materials.

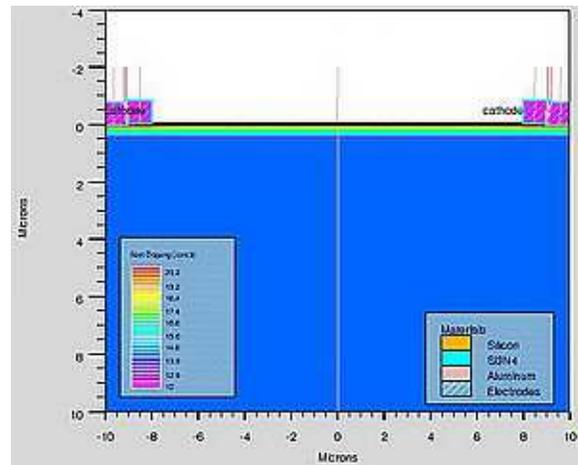
Silvaco TCAD tools can simulate the various aspects of solar cell characteristics. Typical characteristics include collection efficiency, spectral response, open circuit voltage (V_{oc}) and short circuit current density (J_{sc}). Figure 3 described the electrical properties of current density-voltage (J-V) for variable temperature simulation on 50 nm SiO₂ and Si₃N₄ layer deposited on silicon solar cell. While Fig. 4 displayed the J-V characteristics for variable thickness simulation on SiO₂ and Si₃N₄ layer when annealing temperature was fixed to 950°C in second simulation.

DISCUSSION

Figure 1a and 2a shows the colors of silicon substrate region before applying net doping application command. When the 90° incident light was applied on device, there is no reflection beam on silicon substrate region because the device surface is even. If the structure were modified in different surface textured, the incident light on substrate will reflected between device walls^[6]. While the Fig. 1b and 2b shows the solar cell device when applying the net doping color region. The net doping color under SiO₂ and Si₃N₄ coating represents the pn junction developed after phosphorus doping during implantation process of n⁺ layer on silicon substrate.



(a)



(b)

Fig. 2: The cross-section of 10×10 μm² solar cell structure with Si₃N₄ single layer coating

The pn junction can be seen clearly on Fig. 1a and 2a where the horizontal line under SiO₂ and Si₃N₄ coating on silicon substrate. The distance between p-n layers has been extracted using Athena simulator. The SiO₂ layer has a pn junction 0.574 μm meanwhile Si₃N₄ layer has a tiny pn junction of 0.429 μm, both are from 50 nm ARC at 950°C result as shown in Table 4 and 5.

In Fig. 3 and 4, the J_{sc} value is extracted from the curve when voltage is zero. On the other hand, the V_{oc} also can be extracted from the J-V curve when current is zero. In this Fig. 4 clearly shows the current density increased follows voltage value. In J-V curve of Si₃N₄ layer, we can see the current density and voltage values on thickness 90 nm were less compared to other thickness. In overall the range of current density, J_{sc} for SiO₂ layer is around 3.120-3.129 mA cm⁻² and Si₃N₄ layer is approximately to 3.169-3.170 mA cm⁻²,

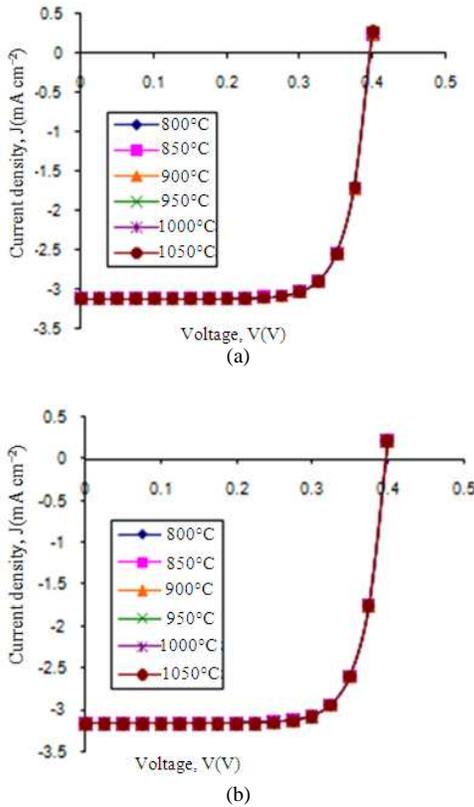


Fig. 3: (a) J-V curve of 50 nm SiO₂ on silicon solar cell for variable temperature. (b) J-V curve of 50 nm Si₃N₄ on silicon solar cell for variable temperature

as shown in Table 2 and 3. This means the J_{sc} of Si₃N₄ layer is higher than SiO₂ layer. Meanwhile the V_{oc} of both layer are nearly to 0.40 V.

In this project, the first simulation has been done running is simulation of variable temperature parameter from 800-1050°C with interval 50°C. For second simulation is variable thickness antireflective coating from 50-90 nm with interval 10 nm. Atlas simulator simulated the pn junction, V_{oc} and J_{sc}, but the Fill Factor (FF) and power conversion efficiency (η) were calculated by using equations below. The fill factor, FF is the ratio of maximum power point, P_m divided by the J_{sc} and V_{oc} and that is:

$$FF = \frac{J_m \cdot V_m}{J_{sc} \cdot V_{oc}} = \frac{P_m}{J_{sc} \cdot V_{oc}} \quad (1)$$

The fill factor is a measure of the realizable power from a solar cell. Typically, the fill factor is between 0.7 and 0.8^[7]. The energy conversion efficiency of solar

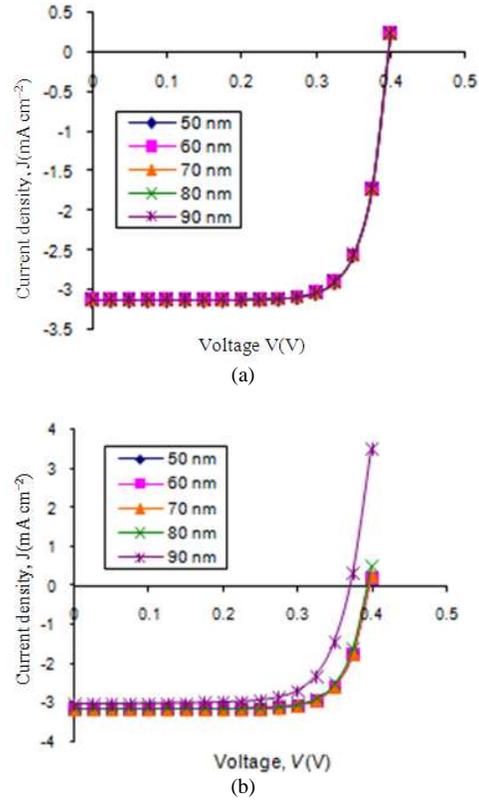


Fig. 4: (a) J-V curve of SiO₂ layer on silicon solar cell for variable thickness. (b) J-V curve of Si₃N₄ layer on silicon solar cell for variable thickness

Table 2: Photovoltaic properties of SiO₂ on silicon solar cell with different Temperature (T) when coating layer is 50 nm

pn junction					
T (°C)	depth (μm)	V _{oc} (V)	J _{sc} (mA cm ⁻²)	FF	η (%)
800	0.4159	0.3978	3.1291	0.757	9.425
850	0.4175	0.3978	3.1290	0.757	9.425
900	0.4253	0.3978	3.1289	0.757	9.426
950	0.5742	0.3977	3.1283	0.758	9.428
1000	0.9047	0.3977	3.1262	0.758	9.426
1050	1.4309	0.3975	3.1200	0.759	9.410

cell, η is the comparison of maximum power point of cell, P_m to input light from source, P_{in}:

$$\eta = \frac{P_m}{P_{in}} \times 100\% = \frac{FF \cdot J_{sc} \cdot V_{oc}}{P_{in}} \times 100\% \quad (2)$$

Earth can received the maximum power from sun is about 1000 W m⁻². So, the input power P_{in} is 1000 W m⁻² with an air mass 1.5 (AM1.5) spectrums^[8]. Table 2 and 3 show the results of photovoltaic properties that have been simulated and calculated for SiO₂ and Si₃N₄ layers on silicon solar cell.

Table 3: Photovoltaic properties of Si₃N₄ on silicon solar cell with different Temperature (T) when coating layer is 50 nm

T (°C)	pn junction				
	depth (μm)	V _{oc} (V)	J _{sc} (mA cm ⁻²)	FF	η (%)
800	0.3876	0.3981	3.1689	0.757	9.552
850	0.3892	0.3981	3.1689	0.757	9.552
900	0.3972	0.3981	3.1689	0.757	9.552
950	0.4290	0.3981	3.1691	0.757	9.553
1000	0.5770	0.3981	3.1695	0.758	9.558
1050	0.9944	0.3980	3.1698	0.758	9.565

Table 4: Photovoltaic properties of SiO₂ on silicon solar cell with different thickness (d) when temperature is 950°C

d (nm)	pn junction				
	depth (μm)	V _{oc} (V)	J _{sc} (mA cm ⁻²)	FF	η (%)
50	0.5742	0.3977	3.1283	0.758	9.428
60	0.5056	0.3977	3.1263	0.758	9.421
70	0.4422	0.3977	3.1245	0.757	9.412
80	0.4264	0.3977	3.1226	0.757	9.405
90	0.4166	0.3977	3.1210	0.757	9.399

Table 5: Photovoltaic properties of Si₃N₄ on silicon solar cell with different thickness (d) when temperature is 950°C

d (nm)	pn junction				
	depth (μm)	V _{oc} (V)	J _{sc} (mA cm ⁻²)	FF	η (%)
50	0.4290	0.3981	3.1691	0.757	9.553
60	0.4137	0.3981	3.1663	0.757	9.544
70	0.1931	0.3980	3.1635	0.757	9.528
80	0.1480	0.3956	3.1612	0.755	9.446
90	0.0875	0.3715	3.0356	0.717	8.083

This simulation was analyzed in different diffuse temperature when the ARC thickness is fixed to 50 nm. From SiO₂ results (Table 2), FF value is approximately 0.758 and efficiency, η is nearly 9.43%. During annealing process, the temperature increased resulted increasing of pn junction depth, but not to V_{oc} and J_{sc} values. Both were decreased slowly when temperature become higher. In this analysis, the optimum temperature for SiO₂ is 950°C because it has higher efficiency, η among others. This could be concluded that the SiO₂ coating was not recommended fabricate at high temperature in annealing process. As for Si₃N₄ result as in Table 3, the calculated FF in range of 0.757-0.758 and efficiency η is around 9.55-9.57%. In annealing process, the temperature increasing constantly follows the increasing of pn junction and J_{sc} while the V_{oc} is decreased slowly. The optimum temperature for Si₃N₄ is 1050°C because has higher efficiency, η among others.

Table 4 and 5 shows the photovoltaic properties of SiO₂ and Si₃N₄ coating layer on silicon solar cell in variable thickness when the annealing temperature was fixed to 950°C. The pn junction depth value for SiO₂ coating layer decreased slowly when thickness of coating layer increased. The calculated FF for SiO₂ coating is approximately 0.758, but the percentage of efficiency decreased when SiO₂ thickness is increased. Details of calculated result were shown in Table 4 and 5.

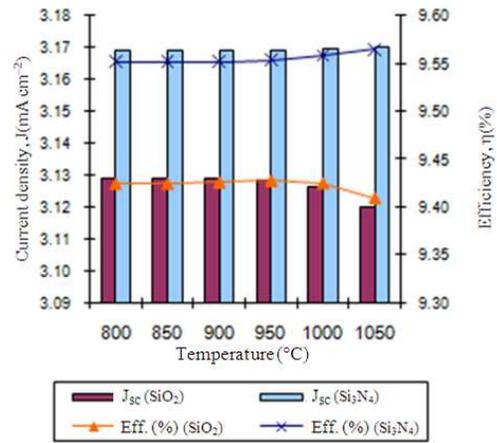


Fig. 5: Graph of current density and photovoltaic efficiency for variable temperature at thickness 50 nm SiO₂ and Si₃N₄ layers coating

For the analysis of Table 5, the pn junction depth become less and less when thickness of SiO₂ coating reached at 70-90 nm. Calculated FF and efficiency values of thickness 50-70 nm were constant. The thickness coating on 80 nm and 90 nm, the FF and efficiency values were decreased. This situation could be concluded that the optimum thickness for Si₃N₄ coating is 50 nm thick. Overall simulation results were illustrated in Fig. 5 that concluded the changes of current density of photovoltaic efficiency for SiO₂ and Si₃N₄ coating in variable temperature. In overall the maximum efficiency that can be reached on SiO₂ and Si₃N₄ layers is 9.428 and 9.553%, respectively. Figure 5 clearly show the current density and photovoltaic efficiency of SiO₂ layer is decreasing, but for Si₃N₄, the both parameter is increasing follows the temperature. In this simulation, the Si₃N₄ material can be proved as an ARC function for solar cell application because it could enhance the J_{sc} and efficiency that could be improved on high temperature.

Figure 6 concluded the changes of current density and photovoltaic efficiency for SiO₂ and Si₃N₄ coating in variable anti-reflective coating thickness. In overall the maximum efficiency that can be reached on SiO₂ and Si₃N₄ layers is 9.428 and 9.553%, respectively. Figure 6 clearly show the current density and photovoltaic efficiency of SiO₂ layer is decreasing, but for Si₃N₄, the both parameter is increasing follows the temperature. But for Si₃N₄ coating, both characteristics were decreased when thickness were become thicker. This simulation proved the fabrication process of single layer SiO₂ and Si₃N₄ coating not required coating to be thick to absorbed more incident light because thick coating could resulted lower efficiency. So, the optimum thickness coating for SiO₂ and Si₃N₄ layer is 50 nm.

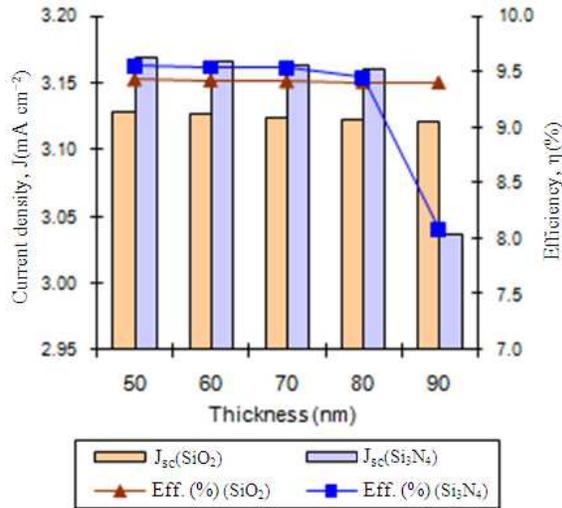


Fig. 6: Graph of current density and photovoltaic efficiency for variable thickness at temperature 950°C SiO₂ and Si₃N₄ layers coating

CONCLUSION

A theoretical study of the ARC on silicon solar cells is made^[9]. The ability of the ATLAS device simulator to accurately a model solar cell characteristic has been shown^[10,11]. The detailed outputs available to the solar cell designer allow for efficient and effective simulation and optimization of even most advanced solar cell designs. Using these tools, the SiO₂ and Si₃N₄ layers silicon solar cell structure was designed by using ATHENA device simulator meanwhile the J-V characteristics for ARC analysis were showing by ATLAS framework. This simulation concentrated on variable ARC thickness deposited on top surface of silicon solar cell at high temperature during annealing process. For SiO₂ results, the FF value are approximately 0.758 and efficiency, η is nearly 9.43%. In annealing process, the temperature become higher resulted increasing of pn junction, but not to open circuit voltage, V_{oc} and short circuit current density, J_{sc} values. The V_{oc} and J_{sc} were slowly decreased when temperature increased. This can be concluded the SiO₂ layer not recommended for high temperature in annealing process. Meanwhile, when SiO₂ coating thickness increased the parameter of pn junction depth, J_{sc} , V_{oc} , FF and η decreased slowly. As for Si₃N₄ result, the calculated FF in range of 0.757-0.758 and efficiency, η is around 9.55-9.57%. In annealing process, the temperature increasing constantly follows the increasing of pn junction depth and J_{sc} , meanwhile the V_{oc} is decreased slowly. At thickness simulation of

Si₃N₄ coating, the value of pn junction depth, J_{sc} , V_{oc} , FF and η parameter were decreased when thickness increased at 10 nm every simulation. The optimum temperature during annealing process of SiO₂ layer is 950°C, while Si₃N₄ layer is 1050°C. For thickness analysis, the optimum antireflective coating of SiO₂ and Si₃N₄ layers are 50 nm both. Solar cell simulation could be useful for time saving and cost consumption. This method also cheaper and faster compared to experimental. So the simulation has some advantages than physical experimental to made decision to fabricate a solar cell.

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