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Research Article

Improved PERC Solar Cell Design by TCAD Simulations

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Abstract: In this work, we aim to identify the performance limiting factors and consequently improve the performance of PERC solar cells through extensive TCAD based device simulation and modelling. Initially, a simplified planar PERC solar cell structure is simulated in Silvaco (Athena/Atlas), where the device geometry is selected according to an experimentally fabricated cell with an efficiency of 17.86%. The J-V curves and solar cell parameters such as J_{sc}, FF, V_{oc} and efficiency (η) of the simulated cell are then fitted to the experimental performance parameters by incorporating relevant models as suggested by the literature. These include: carriers' generation-recombination, mobility, statistics and bandgap narrowing. A good agreement is obtained, where the average percentage difference between simulated and experimental performance parameters is 0.65%. The solar cell performance is then improved to 21.52% by optimising the anti-reflective coating stack composition and thickness, and adding surface texturing. This increase in efficiency is attributed to lower surface recombination and reduced reflection due to light trapping. In addition, a textured front surface enhances the path-length of light, causing it to undergo multiple internal reflections which further increases light trapping, thus increasing J_{sc} by 7.31 mA/cm^2.

Keywords: TCAD Simulation, PERC Solar Cell, ARC, Passivation, Recombination, Surface Texturing.

1. INTRODUCTION

One of the most significant challenges that the world is facing now a days is the ever growing demand of energy due to its major impact on the environment and socio-economic development [1]. So far, renewable energy seems to be a promising way to overcome this issue. Specifically, solar energy, a major source of renewable energy, has a significant potential in fulfilling the future energy needs [2]. In this regard photovoltaics based energy devices, i.e. solar cells, play a leading role in harvesting the abundantly available solar energy [3]. However, despite the enormous potential of electrical energy production through sunlight, solar power contribution in global energy demands is only about 1% [4], as of 2019, which is a very small fraction. To increase the power generation through photovoltaic technologies, the photovoltaic systems must be reliable, more efficient, cost effective, and responsive to the current market demands [2]. To accomplish these goals, the photovoltaic cell architecture needs improvement in terms of reducing manufacturing complexity, cost and related losses while focusing on the optimisation of process steps and their design improvements to enhance the efficiency and reliability.

Passivated emitter and rear cell (PERC) has now become a mainstream device in research and development of solar cells. PERC's first concept was proposed by Blaker et al. at University of New South Wales (UNSW) Australia in 1989 [5,6]. However, it took 25 years for transferring this technology from lab to industry for mass production. Thanks to the passivation layers at front and back, PERC solar cells offer many advantages over the conventional technologies. These include minimising the carrier recombination at the back surface, increased internal reflectivity at rear side resultantly increasing absorption of light and reduced heat absorption leading to increased efficiency (η) [6]. Substantial research is being carried out on PERC solar cells regarding the antireflective coating

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(ARC) [7], passivation, degradation, electrical characteristics, recombination and optical losses etc. However, there is still room for improvement in the design of standard PERC cells. To improve cell architecture and reduce manufacturing complexity, cost, and thoroughly study the loss mechanisms, one way is to adopt computational approach and perform extensive technology computer aided design (TCAD) based device simulations prior to experimentation [8,9].

The present work is aimed to model, optimise, simulate and improve the efficiency of planar PERC solar cell through design modifications using Silvaco TCAD. We have modelled a PERC solar cell and optimised its parameters to fit with the experimentally demonstrated device reported by Kerr et al [10] with an average difference of ~0.65% in J-V parameters from the actual device. We have further modified the device model by adding a texturing on the front surface and additional dielectric layer in the passivation for better performance to improve the efficiency. These modifications have resulted in an efficiency increase from 17.86% to 21.52%.

2. DEVICE SIMULATION

Physics based device simulation tools have become increasingly important in microelectronics research. They are usually known as TCAD, which are used for the simulation of device design and optimisation [11,12]. The physics based device simulation has become significantly important due to two main reasons; firstly, it is quicker and much cheaper than performing experiments, and secondly it gives information that is difficult or sometimes impossible to extract from experiments. Here we have utilised two main tools of Silvaco TCAD, Athena and Atlas, which are physics based simulators that perform process, and 2D/3D device simulations of semiconductor devices respectively. In Atlas module of TCAD, the device simulation problems are specified by defining the physical structure (mesh, substrate, emitter, back surface field (BSF), doping and deposition etc.), models i.e. (of carriers' generation-recombination, mobility, statistics and bandgap narrowing are incorporated) and the bias conditions for which electrical characteristics are to be simulated [11]. We have modelled a planar PERC solar cell and simulated it according to an actual experimentally developed device reported by Kerr et al. [10]. The device was designed by replicating the structure of the actual cell. Its performance was optimised by texturing the front surface and an addition of another dielectric layer of SiO_2 making it a double layer stack. Both these factors have contributed to the efficiency improvement. The device simulation steps are discussed in detail in the following sections.

2.1 PERC Simulation & Modelling

The designed PERC solar cell has a p-type base with a thickness of 300 µm, <100> oriented, 0.3 Ω.cm resistivity, a phosphorous-doped n-type (n+) emitter having a corresponding sheet resistance of 115 Ω/sq. and a 65 nm thick Si_3N_4 passivation layer at front and back. The structure and initial geometry were designed and produced in Athena. It included meshing, defining a substrate, emitter diffusion and the corresponding doping, deposition of Si_3N_4 as a passivation and ARC layer, contact formation and electrode definition. The final structure was then used as an input to Atlas device simulator, whereby (p+) BSF, lifetime, recombination velocities, models, beam (using AM1.5 spectrum) [13] and solutions were initialised. The cell's simulation parameters are given in Table 1.

During simulations, all necessary input parameters were taken into consideration for accurate simulation. Those crucial parameters collectively contributed to develop an accurate model of the planar PERC solar cell. The physics-based simulation models used in our simulations are: Auger to account for auger recombination, Shockley-read-hall (SRH) for SRH recombination, Fermi model for carrier statistics, Klassen [14] for concentration dependent mobility and Schenk [15] for bandgap narrowing. The device physics of these models is discussed in the results and discussion section. The simulations were performed at room temperature i.e. 300 K, using AM1.5 spectrum with effective wavelength range between 300-1400 nm with an angle of 90° (i.e. normal to the cell orientation) [13]. Lastly, the J-V parameters were extracted. The structure of modelled cell is shown in Figure 1.

Table 1. Cell parameters used for the modelling and simulation of planar PERC given in Kerr *et al* [10].

Parameter	Value	Reference	Remarks
Wafer thickness	300 µm	[10]	-
Base resistivity	0.3 Ω.cm	[10]	-
Emitter sheet resistance	100-130 Ω/sq	[10]	Simulated=115 Ω/sq.
Front & back Si_3N_4 thickness	65 nm	[16,17]	-
Recombination velocity at front	1.5×10^5 cm/s	[18,19]	Calculated from eq (1) of [17]
Recombination velocity at back	100 cm/s	[20]	-
Series resistance	0.78 Ω.cm^2	[21,22]	Range=0.3-0.9 Ω.cm^2
Metallization fraction	4%	[10]	-

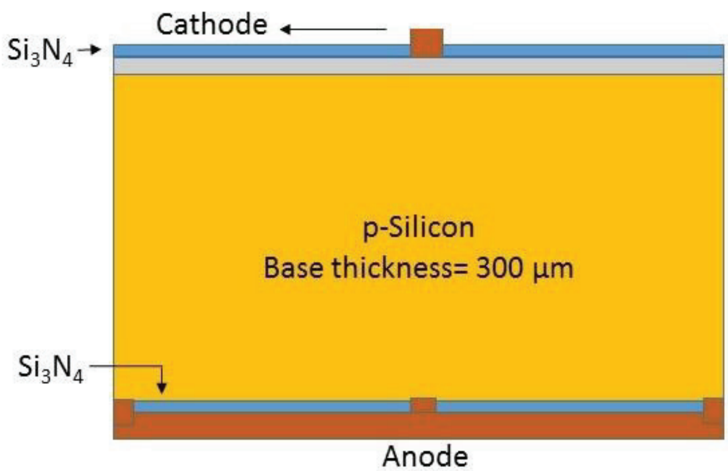

Fig .1. Schematics of the modelled planar PERC

3. RESULTS AND DISCUSSION

3.1 Modelling of Planar PERC

The obtained J-V parameters of both (experimentally demonstrated and simulated) cells are listed in Table 2. The difference between the short circuit current (J_{sc}) is 2.02%, 0.24% between fill factor (FF) and 0.36% between the efficiency (η) while there is no difference between open circuit voltage (V_{oc}). It was found that the parameters of the experimentally demonstrated cell and simulation based cell are in close agreement with a slight average difference of ~0.65% only. This demonstrates the validity of our model and shows that the simulated solar cell model is a closest replica of the actual experimental planar PERC given in Ref. [10].

For further justification of our model, we have fitted the J-V curves of the modelled and experimental PERC as shown in Figure 2. As can be seen that the J-V curves have been closely fitted with a slight difference of ~2% between the experimental and simulated J_{sc} value, where simulated J_{sc} is slightly higher than the experimental value.

Table 2. Relative comparison of the experimental and simulated cell results.

Parameter	Measured [10]	Simulated	% Difference
V_{oc} (mV)	667.3	667.3	0.00%
J_{sc} (mA/cm^2)	33.13	33.8	2.02%
FF (%)	80.70	80.50	0.24%
η (%)	17.80	17.86	0.36%

During simulation, it has been observed that the recombination of carriers affects the cell performance significantly, because when light falls on semiconductor then electron-hole pairs are generated which greatly disturb minority carrier concentration. To return the semiconductor to an

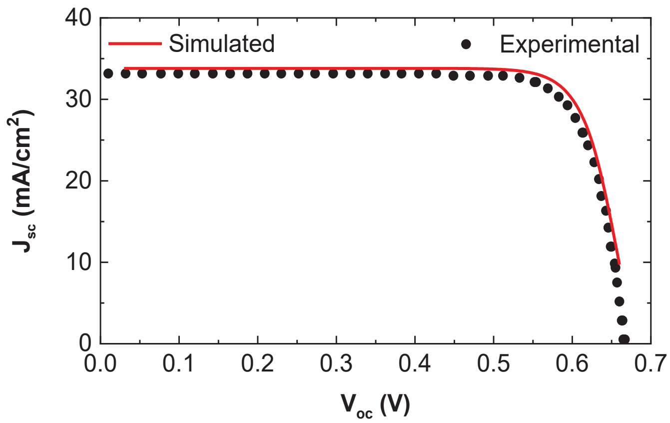

Fig .2. Fitting of J-V curve of the experimental (dotted) and modelled (line) PERC solar cell.

equilibrium, a recombination occurs [11]. If the recombination of carriers occurs before they make it to the electrodes, this causes a huge performance loss. To account for, and suppress recombination and hence to overcome this performance loss, the corresponding recombination models of Auger and SRH were incorporated in the simulation program. The surface recombination at the front side is suppressed by the front passivation layer, while recombination at the rear surface is suppressed by the rear passivation layer as well as by the BSF, which further improves conductivity at the rear side. Suppressed carrier recombination leads to increased V_{oc} and J_{sc}. Furthermore, series resistance was also taken into consideration. Generally, the experimentally determined range of series resistance in cells with PERC topology is 0.3-0.9 Ω.cm^2 [21-22]. Here we have obtained 0.78 Ω.cm^2 as the series resistance value in our modelled cell.

Once the carriers are generated, electric field accelerates them but they lose momentum due to various scattering effects at high concentration, i.e. carrier-carrier scattering, lattice scattering, impurity clustering and scattering as well. Klassen model describes these scattering effects hence accounts for the mobility of both majority and minority-carriers [11,14]. At heavy doping above 10^{18} cm^{-3}, as the doping concentration increases the gap between the valence and conduction band starts decreasing/narrowing. Additionally, temperature and the electron-hole plasma densities in low-doped-regions also cause bandgap narrowing. For this reason, the Schenk model was used which accounts for all these factors [11,15].

It is important to mention that the rear aluminum acts as a back optical reflector in the experimental PERC solar cell. In performing simulations, this factor was incorporated by using "back.refl" command in the beam statement. This way the rear Al acts as a back optical mirror which serves to reflect the transmitted light back inwards the cell for second absorption attempt which has clearly improved the overall performance of solar cells.

3.2 PERC Cell Modification for Improved Efficiency

The fitted device design was considered as a baseline for improving the overall performance of the device. This was done by adding a few design considerations such as the texturing of the front surface, reduction of base thickness, and the replacement of a single nitride (Si_3N_4) passivation as well as ARC layer with a stack. The base thickness was reduced to 180 μm which was initially 300 μm. The front surface was textured with random pyramids to trap more light. A stack of SiO_2 and Si_3N_4 at the front was used instead of Si_3N_4 alone as a passivation layer. The thicknesses of these materials for ARC were selected to be 10 nm and 65 nm for SiO_2 and Si_3N_4 layers respectively. This was done after varying thicknesses over a wide range and studying their corresponding effect on the parameters of the cell. Since the modified PERC has textured front surface, the photogeneration was imported from PV Lighthouse [23], which was not directly possible in Atlas. The photogeneration file

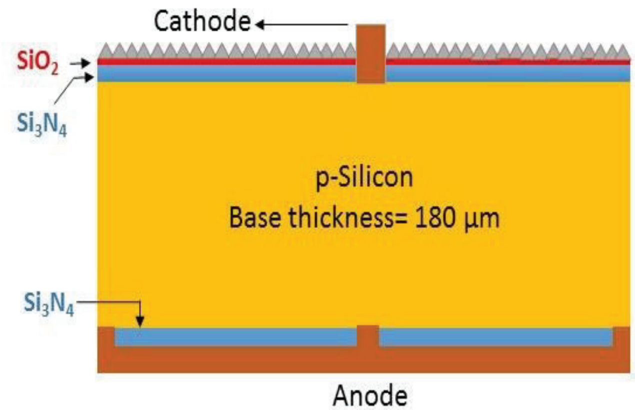

Fig .3. Schematics of the optimized PERC

Table 3: Output parameters of the optimised PERC.

Parameter	Value
V_{oc} (mV)	41.31
J_{sc} (mA/cm^2)	653.26
Fill Factor	79.78
Efficiency (%)	21.52

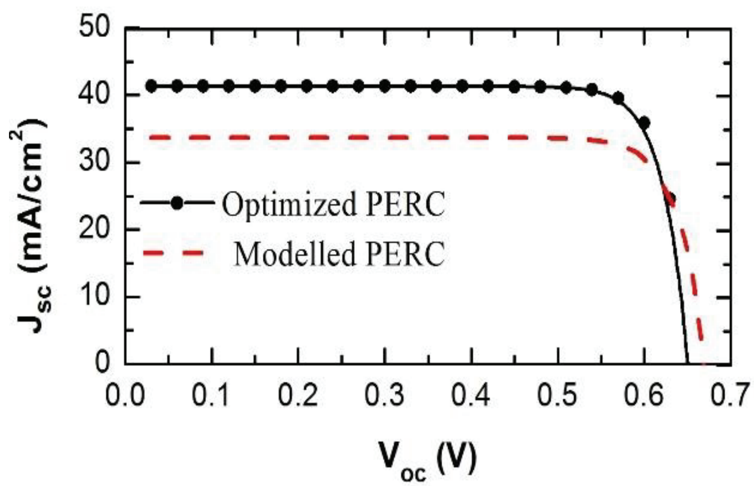

Fig. 4. J-V curves of the modelled (dashed) and optimized (dotted) PERC cell.

was then used as input in the beam statement in Atlas. Structure of the optimised PERC solar cell is shown in Figure 3.

The textured surface of the optimised PERC plays a significant role in improving the performance of the cell. The texturing of front surface enhances the path-length of light, resultantly the light undergoes multiple internal reflections which increases light trapping significantly, thus it minimises reflections from front-side. Besides texturing, a SiO_2/Si_3N_4 stack has further improved light absorption due to their better performance as ARC. The basic purpose of ARC is to obtain zero reflectance by adjusting the refractive indices (n) in such a way that n1 < n2, thereby a phase difference of nπ/2 causes the reflected waves to undergo destructive interference hence they cancel each other, consequently there is no reflection [24]. The stack has suppressed the recombination at the front surface as a consequence of field-effect passivation which shield the charge carriers. Consequently, the electrical characteristics of the modified PERC have been improved in comparison to planar PERC design. The J_{sc} has improved by 7.51 mV which has boosted efficiency by 3.66%. The improved efficiency became 21.52%. The series resistance obtained, was 0.71 $\Omega.cm^2$ which falls within the range as mentioned in Table 1. The output parameters of the optimised PERC are listed in Table 3.

Figure 4 shows the J-V curves of both the modelled and optimised PERC cells, whereby the improvement in Jsc of the optimised PERC cell can be seen.

4. CONCLUSION

A physics based numerical device simulation tool, TCAD, was used to study and improve the design parameters of PERC solar cell. Firstly, a planar PERC solar cell was modelled by following the experimentally demonstrated device parameters. The design of the cell was optimised to fit the J-V parameters with the experimental results. The obtained efficiency of the modelled cell was 17.86%, which had an average difference of 0.65% from an experimentally demonstrated cell. The initial PERC model was then modified by adding texture on the front surface, an additional dielectric layer of SiO_2 in the passivation and reducing the base thickness. These modifications resulted in higher cell efficiency of 21.52%. It is found that the reason for this improvement in efficiency is the texturing of the front surface, which enhances the path-length of light, resultantly increasing light trapping significantly thus minimising reflection from front-side. Besides texturing, an SiO_2/Si_3N_4 stack has further improved light absorption due to its better performance as ARC. Furthermore, the stack has suppressed the recombination at the front surface as a consequence of field-effect passivation which shields the charge carriers, consequently providing better passivation. As a result of all these improvements, the electrical characteristics and the overall efficiency of the modified PERC has been improved in comparison to the planar PERC design.

5. ACKNOWLEDGMENT

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6. CONFLICT OF INTEREST

The authors declare no conflict of interest.

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