Modelling and Simulation Single Layer Anti-Reflective Coating of
ZnO and ZnS for Silicon Solar Cells Using Silvaco Software

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Abstract: In this study, simulated single layer Anti-Reflective Coating (ARC) on silicon solar cell that based
on the refractive index limit of silicon dioxide (SiO₂), zinc oxide (ZnO) and zinc sulphide (ZnS) are presented.
Two simulations of ZnO and ZnS coating were simulated to compare with SiO₂ ARC on silicon solar cell
surface. These simulations carried out with variable coating thickness that is 50, 60, 70 and 80 nm by using
ATLAS simulator. From the simulation obtained, it was found that the value of Vₚ and Jₒ are 397.69 mV
and 15.646 mA/cm², respectively, from silicon solar cell with 0.05 µm SiO₂ coating. For the Fill Factor (FF)
and power conversion efficiency (η) of this solar cell is 0.758 and 4.72% were computed. As for the ARC simulation,
the spectral response of ZnO and ZnS coating was increased around 600 and 700 nm, respectively, which are
able of reducing the refractivity over a wide range of wavelengths compared to SiO₂ increased around
400 nm wavelength. This can be concluded that when the refractive index value is high, the available
photocurrent also can be high in wide range wavelength and more reducing the refractivity. In ARC analysis,
the ZnS coating could perform more efficiency on wide range of wavelength compared to SiO₂ and ZnO ARC.

Key words: Silicon solar cell, SiO₂, ZnO, ZnS, thickness, Silvaco

INTRODUCTION

Silicon is a semi conductor optical material with
relatively high refractive index (Kavalki and Kantari, 2002).
It is an ideal material for solar cell nowadays. Not
only silicon non-toxic, but it is also the second most
abundant element in the Earth’s crust (after oxygen)
posing minimal environmental or resource depletion
issues if used on a large scale. Silicon solar cells have
attracted considerable attention as low cost and high
efficiency solar cells (Minemoto et al., 2007). The material
of pure silicon is shiny. When the light hit the silicon
wafer, it can reflect up to 35% of the sunlight. To reduce
the amount of sunlight lost, an Anti-Reflective Coating
(ARC) is put on the silicon wafer. The most commonly
used coatings are titanium dioxide (TiO₂) and silicon oxide
(SiO₂), though others are used. This case studied of zinc
oxide (ZnO) and zinc sulphide (ZnS) material as an ARC
and to be compared to silicon dioxide coating, SiO₂.
A good ARC is vital for solar cell performance as it
ensures a high photocurrent by minimizing reflectance
(Wright et al., 2005). Unlike many other optoelectronic
devices, solar cells operate at a range of wavelengths,
from 300-1200 nm, which means they need a broadband
ARC. To enhance the short circuit current density (Jₒ)
of solar cells, an ARC is fabricated on the surface of the
solar cells. Si and Si-related materials (such as SiO₂) are of
interest for solar cell work because they can possibly be
used as a surface passivating ARC or as the top cell in an
all-silicon tandem solar cell (Choo et al., 2002). Zinc oxide
(ZnO) has recently received growing attention, as this
material can be produced with superior electrical
cconductivity and optical transparency (Ellmer et al., 2008).
 meanwhile the zinc sulfide (ZnS) is a wide band gap
semiconductor with high refractive index and hence a
promising material for ARC over commercial silicon solar
cells (Gangopadhyay et al., 2004; Nasr et al., 2008).

Traditionally, the simulated electronic devices were
microscopic while solar cells had always been too big to
be modeled (Baudrit et al., 2005). The Silvaco software
deployment is a simulation software tool targeting the area
of electronic design (ATLAS User’s manual et al., 1998).

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One of its major products is the Virtual Wafer Fabrication (VWF) package. This is a large suite of highly sophisticated tools that aid in the design and development of all types of semiconductor and VLSI devices. The Silvaco ATLAS software is already studied in solar cell application (Micheal et al., 2005). ATLAS predicts the electrical characteristics of physical structures by simulating the transport of carriers through a two-dimensional grid. The accuracy of this physically based simulation tool depends greatly on the accuracy of the material parameters used in constructing the solar cell model. Important parameters needed for solar cell modelling in ATLAS include band gap energy, electron and hole state densities, electron and hole mobilities, permittivity, electron affinity, radiative recombination rate and optical parameters. One of the most critical parameters for advanced solar cell modelling is the correct definition of the refractive index, n, and the extinction coefficient, k, for a material. Once a solar cell is simulated in ATLAS, it may be illuminated with a constant wavelength of light or a complex spectrum such as Air Mass Zero (AM0) spectrum, which represents the solar spectrum for earth orbiting spacecrafts. To enter the structure and composition of a solar cell into ATLAS, several parameters must be defined. The most important physical parameters in ARC design are the refractive index (n) and film thickness (d) (Minemoto et al., 2007). By using a numerical analysis, we could calculate the External Quantum Efficiency (EQE) and the performance of the device taking into account many material and structure parameters.

MATERIALS AND METHODS

Silvaco ATLAS is a physically based device simulator that predicts the electrical characteristics that are associated with specified physical design and bias conditions (Baudrit et al., 2005). Physically based simulation is very different from analytical modeling that provides efficient approximation and interpolation but does not provide insight, or predictive capabilities, or encapsulation of the theoretical knowledge.

Modelling solar cell structure: The solar cell that has been chosen for test is made in usual method in VLSI. An orientation silicon wafer of <111> with 50 μm thickness and 1×10^{14} atom cm^{-2} boron concentration was chosen. The 1 μm p-n junction was developed by implant of phosphorus with 1×10^{15} atom cm^{-2} and energy is 110 eV. The diffusion time 300 min and the temperature 900°C are constant. The ATHENA software is used to design the solar cell structure with the area 50×50 μm^2. The next process is applying voltage by using ATLAS simulator to compute open circuit voltage, V_o, and short current density, J_sc. Then the 90° incident light angle is applying on the top of silicon solar cell to trace the reflectance in silicon wafer. The complete virtual solar cell structure shows in Fig. 1.

Simulation of anti-reflective coating: The second step is to simulate the spectral response of variable coating thickness by using ATLAS simulator. The mesh of solar cell has been created to 50x50 μm², then the substrate material is setting up to silicon. The doping concentration of boron is fixed to 1×10^{14} atom cm^{-2} of p type. In this analysis, the beam is fixed to 90° angle and the ARC layer is setting up to variable thickness (50 to 80 nm) to plot the spectral response. Table 1 shows the input data used for ARC analysis simulated by ATLAS simulator. Only using ATLAS simulator can do the ARC simulation by producing spectral response graph to calculate the quantum efficiency of each ARC.

RESULTS AND DISCUSSION

Electrical properties of silicon solar cell: It is described earlier, the solar cell 2D devices have been modelled to compare the electrical properties between silicon solar cell with no SiO₂ and 0.05 μm SiO₂ coating. Figure 1 shows the basic structure of silicon solar cell deposited 0.05 μm SiO₂.
layer when applying 90° incident light. Figure 1 shows the direction of incident light go straight into substrate without reflecting because the surface structure are even or flat, but it does not mean all the photons were fully absorbed. If the surface structure is textured or different angle of incident light before entering the substrate, the direction of light might be reflected.

For the solar cell simulation, the J-V characteristic is shown in Fig. 2. As for the result of $V_{oc}$ and $J_{sc}$ for silicon solar cell structure with SiO$_2$ and no SiO$_2$ coating, it is shown in Table 2. In Table 2 shows the $V_{oc}$ from both is 0.05 μm SiO$_2$ and no SiO$_2$ coating too small referred to the best $V_{oc}$ of silicon solar cell, $V_{oc} = 0.706$ V (Markvart and Castaner, 2003). possibility the area of structure is small, which is 50x50 μm$^2$. It shows the values of $V_{oc}$ and $J_{sc}$ for silicon substrate is higher than 0.05 μm SiO$_2$ coating and the efficiency of virtual cell is decrease about 13.6% when deposited 0.05 μm SiO$_2$ coating. This might be happened the refractive index of SiO$_2$ is lower than 2.0. Figure 2 shows the result computed from solar cell simulation analysis.

**Anti-reflective coating simulation result:** In this study, the ARC analysis has been used four variables thickness of single layer coating with the p-n junction of 1 μm could be simulated. The ARC simulation result is shown in Fig. 3-5, which shows the photocurrent effects of the wavelength on silicon solar cell. The pink line on the top shows the photocurrent from the source and the other lines are the available photocurrent can be absorbed by variable ARC thickness. In Fig. 3 shows there has a empty space or gap between the available photocurrent and source photocurrent lines of SiO$_2$ ARC and this situation might cause of the SiO$_2$ refractive index is lower than 2.0. When the refractive index value is higher, the available photocurrent can be higher in wide range wavelength and more reducing the refractivity. The spectral response of ZnO and ZnS coating are capable of reducing the refractivity over a wide range of wavelengths increase around 600 and 700 nm, respectively (Fig. 4, 5).

The Quantum Efficiency (QE) measurement is one of the most significant characterization tools for solar cells (Schädel et al., 2006). The source photocurrent is the amount of current generated by the light source (ATLAS...
Fig. 6: Graph of External Quantum Efficiency (EQE) for single-layer ARC with variable thickness (a) 50, (b) 60 (c) 70 and (d) 80 nm, respectively on silicon solar cell

User’s Manual, 1998). Available photocurrent is the amount of current absorbed by the semiconductor. Differences between these two photocurrents are due to reflection, transmission or absorption is non-semiconductor materials. The ratio of available and source photocurrents is often known as external quantum efficiency. Figure 6a-d shows the graph of External Quantum Efficiency (EQE) for single-layer ARC with variable thickness (50, 60, 70 and 80, respectively) on silicon solar cell. In overall, the graph shows the SiO₂ is the lowest EQE lines compared to ZnO and ZnS coating. The EQE of ZnO is high increase around 400-700 nm wavelength. Meanwhile, the EQE of ZnS is increasing higher in wide range of wavelength, which is around 600-800 nm wavelength. And this mean the ZnS coating could perform more efficiency on wide range of wavelength. This can be concluded the ZnO layer is the optimum to be a first layer for fabricating multilayer coating solar cell. From the results obtained, it is found that the maximum percentage of EQE, which nearly 99.99% is on 60-80 nm thickness ZnO coating.

CONCLUSION

A theoretical study of the ARC on silicon solar cells is made (Bouhafs et al., 1998). In this study, presented a simulation of single layer ARC on silicon solar cells, based on silicon dioxide (SiO₂), zinc oxide (ZnO) and zinc sulphide (ZnS) coatings by using ATLAS simulator. The ability of the ATLAS device simulator (Micheal and Bates, 2005; Micheal et al., 2005), to accurately a model solar cell characteristic has been shown. 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 basic of silicon solar cell structure was designed by using ATHENA device simulator, meanwhile the J-V characteristics and spectral response for ARC analysis were showing by ATLAS simulator. From the solar cell analysis, it is found the Vₚ is 397.69 mV and Jₚ is 15.646 mA cm⁻², meanwhile the FF and solar cell efficiency is 0.758 and 4.72%, respectively, from 0.05 μm SiO₂ coating. In ARC simulation, the ZnO and ZnS ARC
are capable to reduce the refraction activity because the available photocurrent is increase around 600 and 700 nm for ZnO and ZnS, respectively. And this can be concluded when the refractive index value become higher, the available photocurrent also can be higher in wide range wavelength and capable reducing more refraction on solar cell. For the ARC analysis, the spectral response graph was plotted to evaluate the external quantum efficiency. The percentage of EQE is calculated to compare the differences between coating thickness. From the results obtained the maximum percentage of EQE, which nearly 99.9% is on 60-80 nm thickness ZnO coating. Meanwhile the EQE of ZnS is increasing around 600-800 nm of broad range wavelength. 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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