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## 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 (SiO<sub>2</sub>), zinc oxide (ZnO) and zinc sulphide (ZnS) are presented. Two simulations of ZnO and ZnS coating were simulated to compare with SiO<sub>2</sub> 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 V<sub>oc</sub> and J<sub>sc</sub> are 397.69 mV and 15.646 mA cm<sup>-2</sup>, respectively, from silicon solar cell with 0.05 μm SiO<sub>2</sub> 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 capable of reducing the refractivity over a wide range of wavelengths compared to SiO<sub>2</sub> 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 SiO<sub>2</sub> and ZnO ARC.

**Key words:** Silicon solar cell, SiO<sub>2</sub>, ZnO, ZnS, thickness, Silvaco

### INTRODUCTION

Silicon is a semi conductor optical material with relatively high refractive index (Kavakli and Kantarli, 2002). It is an ideal material for solar cell nowadays. Not only is 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 (TiO<sub>2</sub>) and silicon oxide (SiO), 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, SiO<sub>2</sub>. 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 (J<sub>sc</sub>) of solar cells, an ARC is fabricated on the surface of the solar cells. Si and Si-related materials (such as SiO<sub>2</sub>) 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 (Cho *et al.*, 2002). Zinc oxide (ZnO) has recently received growing attention, as this material can be produced with superior electrical conductivity 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 package 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  $\langle 111 \rangle$  with  $50 \mu\text{m}$  thickness and  $1 \times 10^{14} \text{ atom cm}^{-2}$  boron concentration was chosen. The  $1 \mu\text{m}$  p-n junction was developed by implant of phosphorus with  $1 \times 10^{15} \text{ atom cm}^{-2}$  and energy is 110 eV. The diffuse time 300 min and the temperature  $900^\circ\text{C}$  are constant. The ATHENA software is used to design the solar cell structure with the area  $50 \times 50 \mu\text{m}^2$ . The next

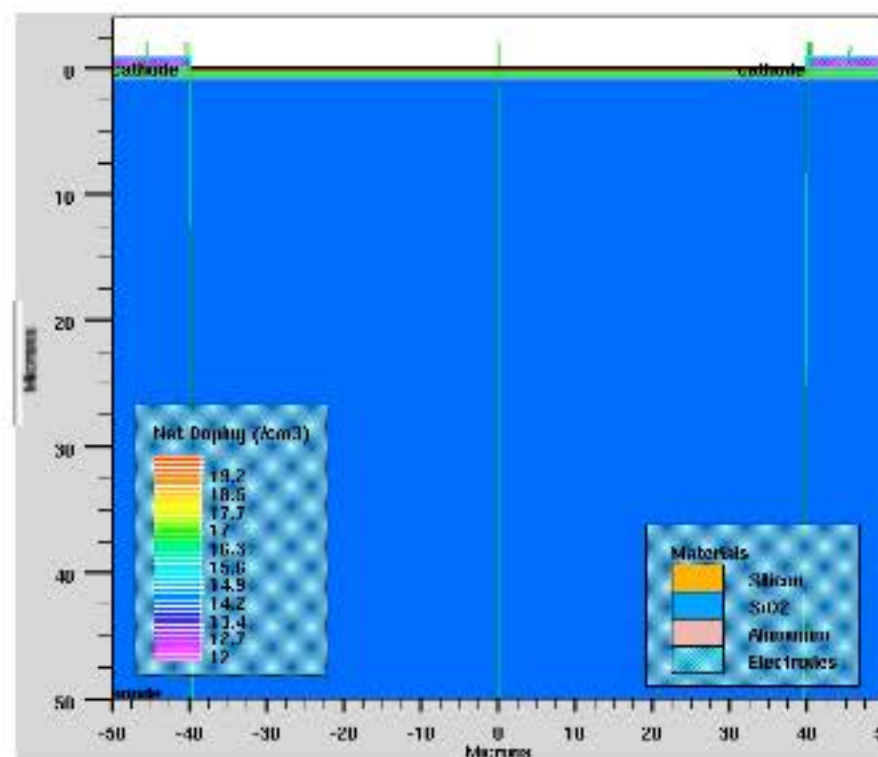


Fig. 1: Silicon solar cell structure with SiO<sub>2</sub> coating when applying 90° incident light

Table 1: The input data of ARC was used in ATLAS simulator (Markvart and Castaner, 2003)

Coating	Refractive index (n)	Thickness (d) (nm)
Silicon oxide (SiO <sub>2</sub> )	1.46	50, 60, 70, 80
Zinc oxide (ZnO)	2.02	50, 60, 70, 80
Zinc sulphide (ZnS)	2.36	50, 60, 70, 80

process is applying voltage by using ATLAS simulator to compute open circuit voltage,  $V_{oc}$  and short circuit 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  $50 \times 50 \mu\text{m}^2$ , then the substrate material is setting up to silicon. The doping concentration of boron is fixed to  $1 \times 10^{14} \text{ atom cm}^{-2}$  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 graph. 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 SiO<sub>2</sub> and  $0.05 \mu\text{m}$  SiO<sub>2</sub> coating. Figure 1 shows the basic structure of silicon solar cell deposited  $0.05 \mu\text{m}$  SiO<sub>2</sub>

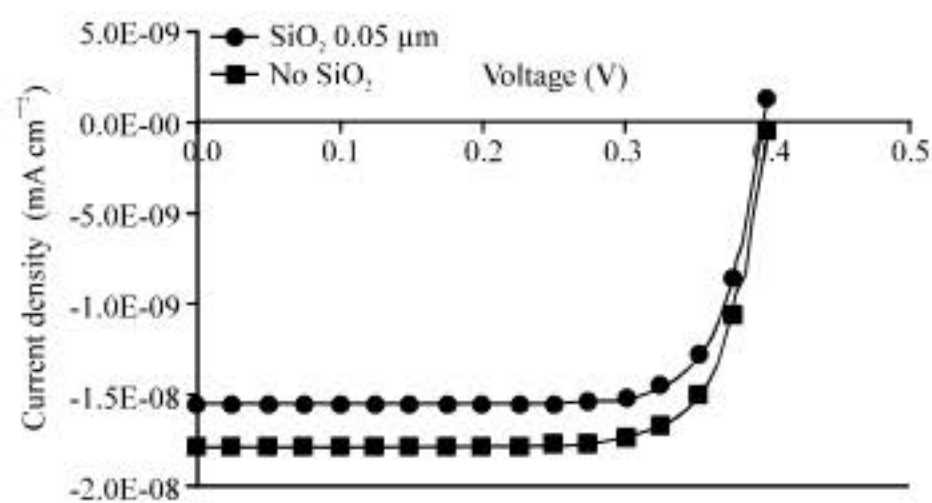


Fig. 2: Graph of J-V characteristics of silicon solar cell with 0.05 μm SiO<sub>2</sub> and no SiO<sub>2</sub> coating

Table 2: The electrical properties of virtual silicon solar cell

Properties	No SiO <sub>2</sub>	0.05 μm SiO <sub>2</sub>
V <sub>oc</sub> (mV)	400.990	397.670
J <sub>sc</sub> (mA cm <sup>-2</sup> )	17.962	15.634
FF	0.758	0.758
η (%)	5.460	4.720

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<sub>oc</sub> and J<sub>sc</sub> for silicon solar cell structure with SiO<sub>2</sub> and no SiO<sub>2</sub> coating, it is shown in Table 2. In Table 2 shows the V<sub>oc</sub> from both is 0.05 μm SiO<sub>2</sub> and no SiO<sub>2</sub> coating too small referred to the best V<sub>oc</sub> of silicon solar cell, V<sub>oc</sub> = 0.706 V (Markvart and Castaner, 2003), possibility the area of structure is small, which is 50×50 μm<sup>2</sup>. It shows the values of V<sub>oc</sub> and I<sub>sc</sub> for silicon substrate is higher than 0.05 μm SiO<sub>2</sub> coating and the efficiency of virtual cell is decrease about 13.6% when deposited 0.05 μm SiO<sub>2</sub> coating. This might be happened the refractive index of SiO<sub>2</sub> 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<sub>2</sub> ARC and this situation

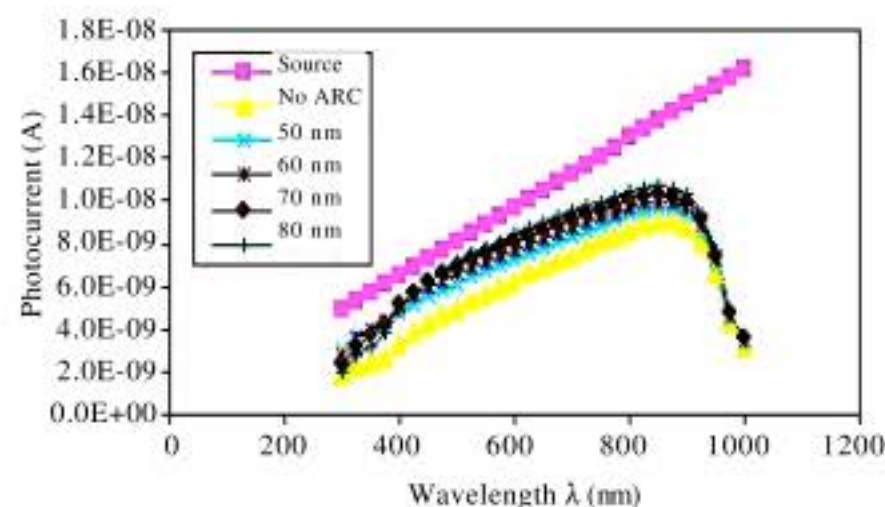


Fig. 3: Graph of spectral response of variable thickness SiO<sub>2</sub> ARC (d = 50 ~ 80 nm)

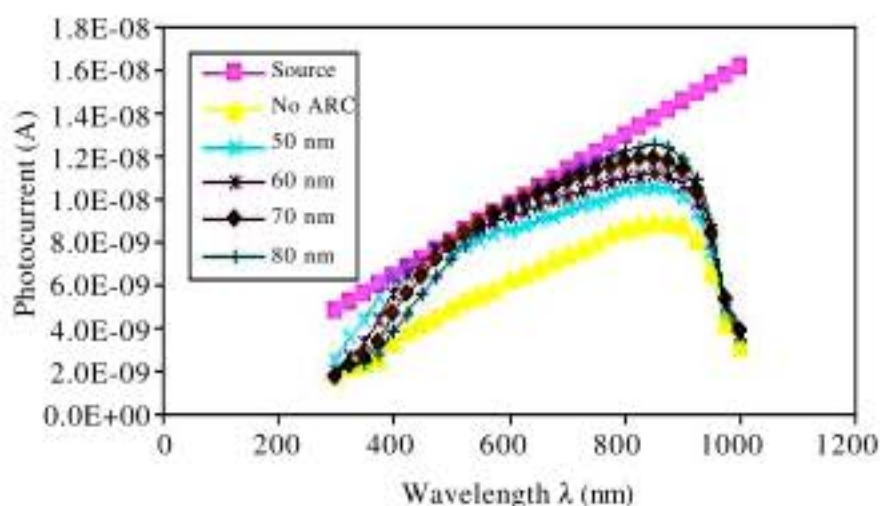


Fig. 4: Graph of spectral response of variable thickness ZnO ARC (d = 50 ~ 80 nm)

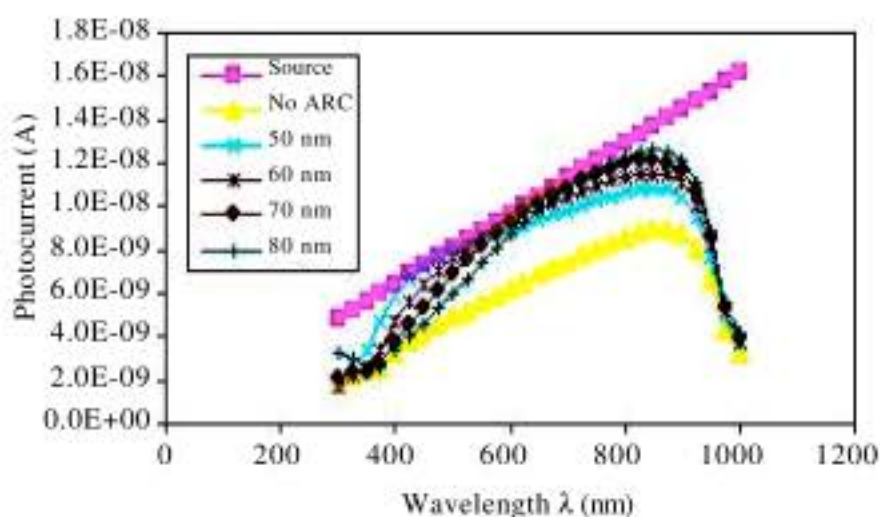


Fig. 5: Graph of spectral response of variable thickness ZnS ARC (d = 50 ~ 80 nm)

might cause of the SiO<sub>2</sub> 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

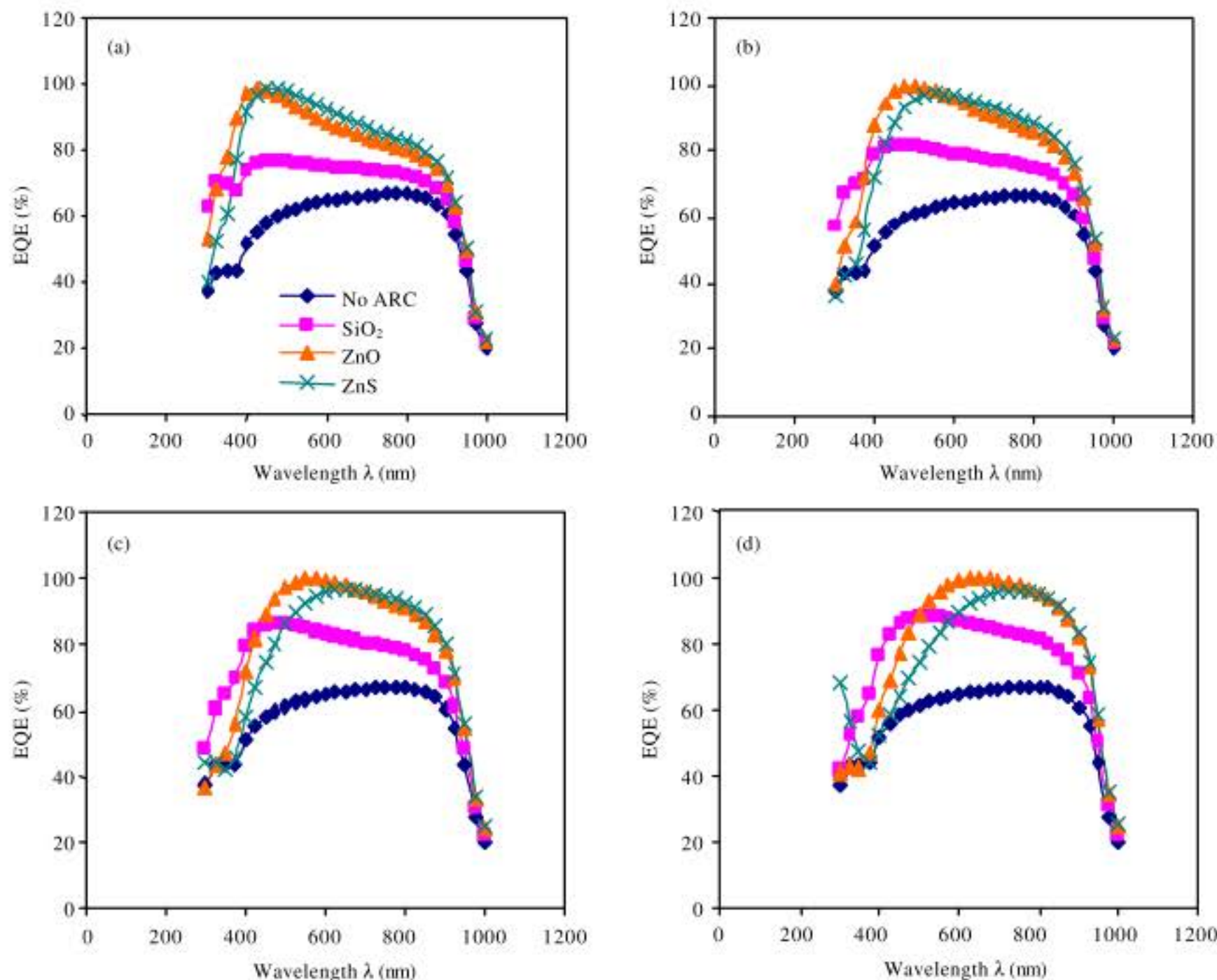


Fig. 6: Graph of External Quantum Efficiency (EQE) for single-layer ARC with variable thickness (a) 50, (b) 60 (c) 70 and (d) 80 nm, respectively on silicon solar cell

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 SiO<sub>2</sub> 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 (SiO<sub>2</sub>), 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 V<sub>oc</sub> is 397.69 mV and J<sub>sc</sub> is 15.646 mA cm<sup>-2</sup>, meanwhile the FF and solar cell efficiency is 0.758 and 4.72%, respectively, from 0.05 μm SiO<sub>2</sub> coating. In ARC simulation, the ZnO and ZnS ARC

are capable to reduce the refractivity 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 refractivity 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 coatings thickness. From the results obtained the maximum percentage of EQE, which nearly 99.99% 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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