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Numerical Modelling of High Efficiency ZnO/GaAs Solar Cell Using Single Layer Anti-Reflective Coating (SLARC)

Zinc oxide, ZnO, and gallium arsenide, GaAs, are a pair of materials that can build a good structure for a solar cell device as n-type and p-type, respectively. Both materials were promising good efficiency due to their optical and electrical properties in semiconductors. For that, the thickness of the material of SLARC was calculated using a formula to investigate the efficiency between 250 nm and 1200 nm of wavelength. The efficiency of the n-ZnO/p-GaAs cell without using ARC recorded 17.76%, and applying SLARC of silicon dioxide, SiO_2, on top of the cell showed 19.62% using Personal Computer 1-Dimensional (PC1D) simulation.

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1. Introduction

Energy is the most fundamental element required to accomplish all human tasks and the most universal indicator of all human and natural labour [1]. Without restrictions, the rate at which natural resources are being used may soon become extinct. Renewable energy like solar, wind, hydropower, geothermal, and many more began to be used as the main source of energy. Recently, solar energy has been used globally to gain energy, and also numerous researchers have studied the solar cell to improve and increase the efficiency.

A solar cell is a device that can directly convert solar energy to electricity. Sunlight is composed of photons, which can be thought of as “packets” of energy [1]. The creation of a photovoltaic effect results from the energised electrons moving from the negative terminal to the positive terminal. First-generation silicon solar cells, which are produced and utilised on a massive scale, are classified as either monocrystalline or polycrystalline silicon solar cells [2]. However, the researcher came out with a new structure of the solar cell by using other materials to study the photoelectric conversion efficiency. Every material has its properties and characteristics that can lead to different results, which can help to study and identify the best materials that can be used in solar cell devices. In the photovoltaic industry, silicon is the common material that has been used, as it gives the best efficiency. However, over recent years, zinc oxide has been widely used in this technology industry. ZnO is exploited in this industry due to its wide and direct band gap and relatively high conductivity, which can promise high efficiency. The material has a direct band gap energy of 3.289 eV and a refractive index of 2.00. Furthermore, ZnO can be available at low cost. ZnO coating may be utilised as an active layer for single heterojunction solar cells in addition to being an antireflective layer. It can partner with other p-types, such as GaAs [3]. Among III-V semiconductors, GaAs has remained useful as a semiconductor material, widely being used in optoelectronic and microelectronic devices [4]. It has a direct band gap of 1.42 eV, which is suitable for optoelectronics. Although a large number of research studies on ZnO/Si heterojunction solar cells have already been published, only a small number of tests have shown that, when correctly optimised and built, ZnO/GaAs exhibits superior electrical quality and efficiency [4].

GaAs is an ideal material for matching with ZnO because their bandgap is direct and wide, respectively, which can make ZnO act as a transparent conductive oxide (TCO). Proper formation of ZnO/GaAs helps to reduce surface recombination and improves carrier collection. Furthermore, GaAs has a higher temperature tolerance than Si, which allows ZnO/GaAs solar cells to continue to produce high power at high temperatures. Temperature plays a crucial role in the efficiency influenced by the operating temperature of the cell. Furthermore, the primary objective shared by all researchers is to

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maximise efficiency in their work. On the other hand, light can reflect back, meaning that when sunlight strikes a solar cell, the majority of the light will be bounced back into the air, which may result in low photon absorption. To overcome this problem, anti-reflective coating (ARC) was widely used in the photovoltaic industry to reduce the reflectance of light, which directly can help to maximise the efficiency of solar cells. Some researchers were coming up with an idea of using multilayer anti-reflective coating (MLARC) as it will help to capture more light; however, the design and calculation will be more complex and increase the cost. Thus, single-layer anti-reflective coating (SLARC) will make the design simpler and economically viable. Also, it is possible to maximise the efficiency and reduce the reflectance by using a well-designed SLARC.

The solar cell's illuminated surface is covered with a thin coating of dielectric material known as an ARC layer, which improves light transmission and lowers optical losses brought on by reflection [5]. Additionally, the choice of ARC's materials is important, as every material has its own characteristics that can contribute to the increment of the absorption of photons. The optimum values for thickness and refractive index of ARC for each material were calculated at specified wavelengths. The arrangement for refractive index of ARC needs to be lower than the refractive index of n-type material, which is ZnO, to produce destructive interference between these layers, which can indirectly reduce the reflection of light. Researchers previously focusing on optimisation value for the parameters of solar cells without using any ARC using Atlas Silvaco software and experimental methods; meanwhile, in this study, the efficiency of the solar cell was discovered by using Personal Computer 1-Dimensional (PC1D) simulation software. In this study, n-ZnO/p-GaAs solar cell was used as a solar cell device to determine the efficiency with and without applying ARC on the top solar cell as shown in Figure (1). Single layer of anti-reflective coating (SLARC) intends to be utilised in specified wavelength ranges, which are 250 nm–1200 nm using PC1D.

2. Simulation Part

For the ZnO/GaAs solar cell, the effects of three different ARC types - SiO_2, ZnO, and silicon nitride (Si_3N_4) as well as those without ARC were examined independently in this work. Hashmi et al. carried out a simulation with wavelengths ranging from 250 to 1200 nm to determine the ideal wavelength needed for solar cell ARC design. The effectiveness of the solar cell using this range of wavelengths is because it's covering the range of the solar spectrum, which can help to reduce the reflection. The required thickness for each range of wavelength can be calculated by using

$$d = \frac{\lambda_0}{4 \, X \, n_{ARC}} \quad (1)$$

where d is thickness of ARC, and λ_0 is a certain wavelength's anti-reflection coating's refractive index (n_{ARC}). From Hashmi et al., n_{ARC} for various ARCs can be obtained from 250 to 1200 nm of wavelength to input into Eq. (1) for finding optimum thickness.

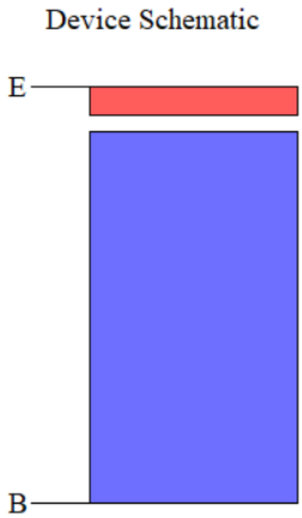

Fig. (1) Schematic diagram of ZnO/GaAs solar cell

These parameters were used in PC1D to determine the simulation's maximum power output (P_{max}), open circuit voltage (V_{OC}), and short circuit current (I_{SC}). The output can be used to calculate the fill factor (FF) and efficiency of the solar cell. Indicators like the fill factor (FF) are commonly used to assess how efficient solar photovoltaic modules are [6]. It can be calculated by using this formula:

$$FF = \frac{P_{max}}{I_{SC} \, X \, V_{OC}} \quad (2)$$

It's also important to keep in mind that the energy level alignment of the hole transport layer and the photoactive layer system effects the fill factor in heterojunction cells. Additionally, the following formula may be used to assess the efficacy of a solar cell:

$$\eta = \frac{I_{SC} \, X \, V_{OC} \, X \, FF}{P_{in}} \quad (3)$$

where η represent is the efficiency of the solar cell and P_{in} is the power input into the cell from sunlight. which can be calculated by constant intensity multiplied with device area of the solar cell.

The researcher used a computer modelling method before producing the actual one to make sure the solar cell was able to perform maximally. In this paper, PC1D was used to numerically investigate the efficiency of a ZnO/GaAs solar cell with and without applying an ARC on the top of the solar cell. Due to its ability to model the behaviour of semiconductor-based photovoltaic devices in one dimension (axial symmetry), PC1D is a well-known piece of software among solar researchers [10]. Besides that, it is widely used in academia and research areas due to its free

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availability and proven reliability in the photovoltaic area. PC1D provides key parameter performance such as short-circuit current (I_{SC}), open-circuit voltage (V_{OC}), and maximum power output (P_{max}) which can be used to determine the optimization of solar cell by calculating fill factor and efficiency.

Table (1) Parameters of ZnO and GaAs solar cell using PC1D simulation

Parameter	Value	Ref.
DEVICE		
Device area	110 cm^2	
Surface texturing	None	
Surface charge	None	
Exterior front reflectance	10%	[6]
Exterior rear reflectance	None	
Internal optical reflectance	None	
REGION 1		
Thickness	0.2μm	[7]
Material	ZnO	
Dielectric constant	7.9	
Band gap	3.289 eV	
Intrinsic concentration at 300K	$1.1x10^{-9}$	
Refractive index	2.00	
N-type background doping	$1x10^{18}$ cm^{-3}	
Bulk recombination, $\tau_n = \tau_p$	1000μs	
REGION 2		
Thickness	100μm	[7]
Material	GaAs	
Dielectric constant	13.18	
Band gap	1.424 eV	
Intrinsic concentration at 300K	$1x10^9$	
Refractive index	3.66	
P-type background doping	$5x10^{15}$ cm^{-3}	[8] [9]
Bulk recombination, $\tau_n = \tau_p$	1000μs	
EXCITATION		
Excitation from	one-sun	
Excitation mode	Transient, 16 time steps	
Temperature	25°C	
Base circuit	-0.8 to 0.8 V	
Collector circuit	Zero	
Primary light source	Enabled	
Constant intensity	0.1 W cm^{-2}	
Spectrum	AM1.5G	
Secondary light source	Disabled	
Other parameters are default by PC1D		

In this paper, the device area was set up to 110 cm², and exterior front reflectance is 10%. ZnO as n-type was set up in REGION 1 with the intrinsic concentration $1.1x10^{-9}$, and n-type background doping is $1x10^{18}$ cm^{-3}. In the meanwhile, REGION 2 was set up as the p-type of GaAs form. The values of intrinsic concentration and p-type background doping are $1x10^9$ and $5x10^{15}$ cm^{-3} individually. This simulation was a study under the solar spectrum, AM1.5G, with "ONE-SUN" for the excitation mode. Other parameters for both region, device, and excitation are default as shown in table (1) and Fig. (2). The performance of the solar cell can be influenced by the thickness of the substrate and ARC, with increasing thickness potentially assisting in the absorption of more photons.

However, bulk recombination may rise if the substrate is very thick. Thus, Manoua et al. [3] has studied the optimisation value for the thickness for ZnO and GaAs, which are 0.2 and 100, respectively, that were used in this study.

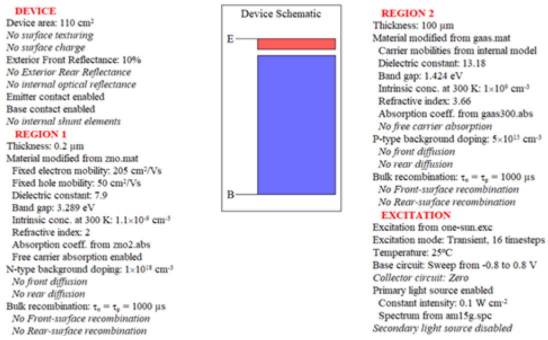

Fig. (2) The settings of the DEVICE and REGION in PC1D

3. Results and Discussion

The solar cell without using any ARC were simulated using PC1D that can produce maximum power output (P_{max}), open circuit voltage (V_{OC}), and short circuit current (I_{SC}) as a result. Using these parameters, the fill factor and efficiency can be calculated using Eq. (2) and (3) respectively. Table (2) shows the result for the n-ZnO/p-GaAs solar cell without applying any ARC on the top of it, and Figure (3) is the graph I-V for the solar cells. The obtained photovoltaic parameters for the n-ZnO/p-GaAs solar cell is 3.253A, 1.954W, and 0.7130V for short-circuit current (I_{SC}), maximum power output (P_{max}), and open-circuit voltage (V_{OC}), respectively which can calculate the efficiency of the device approximately 17.76%. However, Derbali L., (2022) achieved 8.31% for the efficiency of the reference n-ZnO/p-GaAs solar cell in an experimental way. Also, Manoua et al. [3] successfully came out the efficiency of as much as 21.21% using Atlas Silvaco software. These slight differences between the efficiency due to the usage of various software. Kowsar et al. [11] were explained the various software that can be used in the solar cell simulation method, which draws attention to the differences in modelling and computational techniques used by various simulators, which may result in differences in the anticipated performance of solar cells.

The I-V curve in Figure (3) is essential for evaluating solar cell efficiency. According to the graph, when the voltage is zero, the current appeared to be around 3.10A-3.20A, which is known as the maximum current that can appear under the illumination or short-circuit current (I_{SC}). However, the voltage at which the current drop to zero is around 0.70V-0.75V. This is the maximum voltage that can be produced when no current flows. The transition of

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power production to diode-like behavior is represented by the abrupt dip close to V_{oc}. Good performance is shown by the curve's high fill factor (FF), which can lead to high efficiency. Referring to the graph I-V in Figure (3), at a current and voltage of 3.01A and 0.65V, respectively, it started to drop continuously, and this phenomenon called as maximum power point (MPP). The empirical-based PV models attain more accuracy in the region of the MPP because they are curve-fitting derivatives of the graphical features of the I-V curve and require fewer fitting parameters [12].

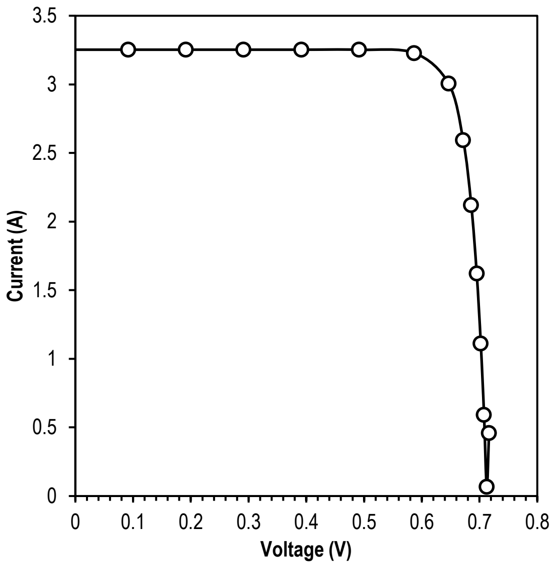

Fig. (3) I-V curve for ZnO/GaAs solar cell without ARC

However, this solar cell device can be improved by applying the layer of ARC on the top of the device. In this paper, SiO_2, Si_3N_4 and ZnO were chosen to be the material of SLARC due to their characteristics and refractive index, which is lower than the refractive index of n-ZnO. Destructive interference will happen if the refractive index of the ARC is lower than the p-n material. Table (3) shows the result of efficiency for each material of ARC on the top of ZnO/GaAs solar cell in the range of wavelengths from 250nm to 1200nm.

Based on table (3), different refractive index and wavelengths is leaded to different values of thickness. Based on Eq. (1), thickness depends on the refractive index and wavelength of the material. According to the result, SiO_2 recorded the highest efficiency among the materials. In the range of wavelengths in SiO_2, the highest efficiency is 19.62% at 600 nm. The values of short circuit current (I_{SC}), maximum power output (P_{max}) and open circuit voltage (V_{OC}) are 3.551A, 2.158W, and 0.7152V, respectively. Meanwhile, the wavelength at 250 nm recorded the lowest efficiency for SiO_2 as an ARC, which is 18.34%. The second highest efficiency is ZnO, which is 18.08% at 700 nm with 3.311 A, 1.989 W, and 0.7134 V as I_{SC}, P_{max}, V_{OC} respectively. Lastly, ZnO was followed by Si_3N_4 which is 17.59%. However, Si_3N_4 recorded 17.59% at four different wavelengths, which are 900, 1000, 1100, and 1200 nm. However, the last three values of wavelength produced the same value for I_{SC}, P_{max}, V_{OC}. This happened because of its bandgap, meaning it can absorb the light with wavelengths below 1000 nm. The inability of photons with wavelengths longer than 1100 nm to drive electrons from the valence band to the conduction band is the reason why silicon is not an effective light absorber. Wavelengths over 1000 nm were excluded from consideration of reflection values since light reflected at the solar cell's back and not absorbed by the silicon dominates this region of the reflection spectrum [13].

Figure (4) shows the graphs for short-circuit current (I_{SC}) and open-circuit voltage (V_{OC}), respectively, that explain the relationship between current and voltage for each material of ARC. As can be seen, SiO_2's graph is the highest for both graphs, which can be concluded to mean that it's more efficient compared to other materials to be a SLARC. In terms of thickness optimisation and spectrum responsiveness, SiO_2 can outperform ZnO and Si_3N4, despite their closer refractive indices to the ideal.

By comparing the efficiency of ZnO/GaAs solar cells without and with ARC layers, it is demonstrated that the ARC layer affects solar cell efficiency [14]. ZnO/GaAs solar cell without using ARC promising good efficiency, but there's still reflectance of light that can be reduced to increase the percentage of efficiency. The analysis of the short circuit current and cell efficiency specifically demonstrates the advantageous impact of ARC [15]. However, the refractive index of the ARC needs to be accentuated; otherwise, it will reflect more light and indirectly decrease the efficiency. By applying a low-refractive-index anti-reflection coating (ARC) layer to the front surface, this issue will be lessened [15].

4. Conclusion

In the conclusion, the simulation of SLARC on the n-ZnO/p-GaAs solar cell device using PC1D simulation with different refractive index and thicknesses of ARC in the range of 250 nm–1200 nm produced different outputs. Out of three materials that were used to study the ARC, SiO_2 achieved the highest efficiency at a wavelength of 600 nm, which improved the efficiency of the solar cell without applying ARC from 17.68% to 19.38%. Meanwhile, ZnO recorded the lowest efficiency with 16.10% at 300 nm. This occurred because destructive interference cannot occur with a refractive index greater than n-ZnO (n = 2.00) at a wavelength of 300 nm. From the result, ARC played a vital role in improving the efficiency of the solar cell.

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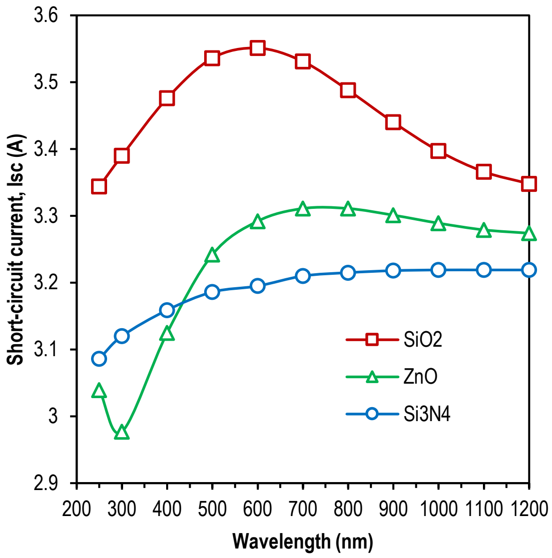
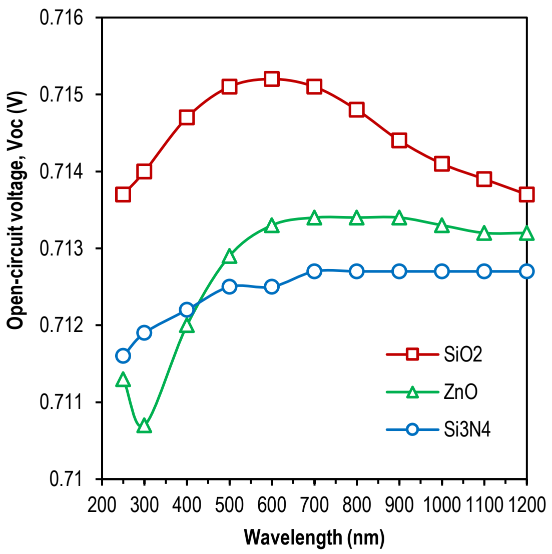


(a)



(b)

Fig. (4) (a) Current vs. wavelength, and (b) voltage vs. wavelength for ZnO/GaAs with SLARC

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Table (2) Data of PC1D simulation for ZnO/GaAs without ARC

Short-circuit current, I_{SC} (A)	Maximum power output, P_{max} (W)	Open-circuit voltage, V_{OC} (V)	Fill Factor, *FF*	Efficiency, *η* (%)
3.253	1.954	0.7130	0.8425	17.76

Table (3) Data of SLARC of n-ZnO/p-GaAs solar cell

		SiO_2					
Wavelength, λ (nm)	Refractive index, n	Thickness, d (nm)	I_{SC} (A)	P_{max} (W)	V_{OC} (V)	Fill Factor, FF	Efficiency, η (%)
250	1.520	41.12	3.344	2.017	0.7137	0.8451	18.34
300	1.510	49.67	3.390	2.050	0.7140	0.8469	18.64
400	1.500	66.67	3.476	2.109	0.7147	0.8489	19.17
500	1.482	84.35	3.536	2.148	0.7151	0.8495	19.52
600	1.480	101.35	3.551	2.158	0.7152	0.8497	19.62
700	1.474	118.72	3.531	2.145	0.7151	0.8495	19.50
800	1.473	135.78	3.488	2.117	0.7148	0.8491	19.25
900	1.472	152.85	3.440	2.085	0.7144	0.8484	18.95
1000	1.471	169.95	3.397	2.055	0.7141	0.8471	18.68
1100	1.470	187.07	3.366	2.033	0.7139	0.8460	18.48
1200	1.469	204.22	3.348	2.020	0.7137	0.8454	18.36
		Si_3N_4					
Wavelength, λ (nm)	Refractive index, n	Thickness, d (nm)	I_{SC} (A)	P_{max} (W)	V_{OC} (V)	Fill Factor, FF	Efficiency, η (%)
250	2.289	27.304	3.086	1.860	0.7116	0.8470	16.91
300	2.167	34.610	3.120	1.880	0.7119	0.8464	17.09
400	2.070	48.309	3.159	1.902	0.7122	0.8466	17.29
500	2.030	61.576	3.186	1.917	0.7125	0.8445	17.43
600	2.020	74.257	3.195	1.922	0.7125	0.8443	17.47
700	2.003	87.369	3.210	1.931	0.7127	0.8441	17.55
800	1.996	100.200	3.215	1.933	0.7127	0.8436	17.57
900	1.991	113.009	3.218	1.935	0.7127	0.8437	17.59
1000	1.985	138.539	3.219	1.935	0.7127	0.8434	17.59
1100	1.985	138.539	3.219	1.935	0.7127	0.8434	17.59
1200	1.983	151.286	3.219	1.935	0.7127	0.8434	17.59
		ZnO					
Wavelength, λ (nm)	Refractive index, n	Thickness, d (nm)	I_{SC} (A)	P_{max} (W)	V_{OC} (V)	Fill Factor, FF	Efficiency, η (%)
250	2.388	26.173	3.039	1.833	0.7113	0.8480	16.66
300	2.404	31.198	2.977	1.795	0.7107	0.8484	16.32
400	2.114	47.304	3.125	1.882	0.7120	0.8458	17.11
500	1.968	63.516	3.242	1.948	0.7129	0.8428	17.71
600	1.913	78.411	3.292	1.977	0.7133	0.8419	17.97
700	1.883	92.937	3.311	1.989	0.7134	0.8421	18.08
800	1.864	107.296	3.311	1.988	0.7134	0.8391	18.07
900	1.851	121.556	3.301	1.982	0.7134	0.8387	18.02
1000	1.841	135.800	3.289	1.975	0.7133	0.8420	17.95
1100	1.833	150.027	3.279	1.970	0.7132	0.8424	17.91
1200	1.826	164.294	3.274	1.967	0.7132	0.8424	17.88

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