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Evaluation of the Effectivenes of TiO_2 Antireflection Coating for Solar Cell

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Abstract
This study presents the effects of anti-reflection coating (ARC) thickness and operating temperature on the reflectance, open circuit voltage, short circuit current and efficiency of $GaAs$ solar cells with and without TiO_2 ARC. The work is conducted in the COMSOL Multi-physics environment where the semiconductor and electromagnetic wave frequency model were implemented. The results showed that, the ARC thickness at 80nm is able to reducing the reflectance from 32% to 5%, which led to the overall efficiency of the solar cell to increase from 19% to 25%. Moreover, at high temperature of 70 ℃ the thermal voltage and the rate of charge recombination increase leading to decrease in the open circuit voltage from 1.030V to 1.015V resulting in the decrease of efficiency to 23%. The effectiveness of the ARC in enhancing the solar cell efficiency is clearly illustrated in this work. Thus, more efficient panels can be manufactured with the use of ARC.

Keywords: Anti-reflection coating, COMSOL Multi-physics, Efficiency, Reflectance, Solar cells

INTRODUCTION
Renewable energy sources have become more popular in recent years due to the reduction in fossil fuel reserves and growing global warming. Among the alternative energy sources solar energy is the third widely used because of its availability (Noman *et al.*, 2022). The abundant solar energy is converted to electric energy using photovoltaic cell which works based on photoelectric effect. Different materials such as silicon, amorphous silicon (a-Si), gallium arsenide (GaAs), copper indium selenium (CIS), copper indium gallium selenium (CIGS) has being used for solar cells fabrication(Leem *et al.*, (2014); Atwater and Polman, (2010)).

Research development in enhancing the efficiency of the solar cell, started from the first and second generation that comprise silicon and thin film solar cell respectively. Although silicon solar cells are used in large scale because of its abundance, low cost and nontoxic. However, low efficiency recorded from the first generation shifted the PV technology to second (semiconductor thin film) generation which comprise $CIGS, GaAs, a-Si$ etc (Ji *et al.*, 2022). In recent years, the limited performance and stability of the previous generations yielded the third generation of PV technology (Michael and Niu, 2022). These limitations were utilized in order to look for the new solar cell materials that are more efficient and favorable. The third-

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generation solar cells includes tandem solar cells, organic polymer solar cells, hetero-junction solar cells, dye-sensitized solar cells, quantum dot solar cells etc.

In continuation of the solar cells efficiency improvement, researchers are much concerned about the photoelectric conversion efficiency (Segbefia, Imenes and Sætre, 2021). However, there are many mechanisms that affect the efficiency of solar cell when expose to outdoor environment. Reflection loss due to surface reflection and the heat generation caused by high-energy charge carriers in the short wavelength range are among the major mechanisms that hinder the efficiency of solar cells (Brahma, Baruah and Sarmah, 2018). Anti-reflection coating (ARC) is the most effective among the strategies of reducing reflection lost and heat generation from the front surface of the solar cells (Mandong and Uzum, 2021). Different materials have been explored to develop the ARC with high performance, such as silicon dioxide (SiO_2), magnesium fluoride (MF_2), aluminium dioxide (AlO_2), titanium dioxide (TiO_2) etc. High refractive index of 2.7, nontoxic, abundancy, low cost, low absorption in visible region and self-cleaning properties, made the TiO_2 more acceptable than other materials. For reflection, its mainly use the principle of destructive interference to control the Fresnel reflection loss caused by the propagation of light in different media (ARC and solar cell). However, the effect of ARC thickness and temperature rise on solar cell efficiency is yet to be fully evaluated. Therefore, evaluating the optical and electrical properties of the coated solar cells is of great significance for obtaining effective ARCs with outstanding performances.

Leem et al., (2014) reported that, the optical reflection properties of single-junction solar cells with 50 nm thick nanostructure TiO_2 ARC could reduce reflection to 6.2% in the wavelength range of 350-900 nm at incident light angles of $3^0 - 80^0$ compared to cells without ARC. Jha et al., (2018) reported the reduction of the maximum efficiency by 15% and 16% from the clean and dusty silicon solar panel without ARC when the temperature rises from $40°C\ to\ 50°C$. Brahma et al., (2018) carried out the experimental and simulation work to evaluate the effect of temperature on electrical parameters of solar cells without coating. The result have shown that, the temperature raised from $25°C\ to\ 40°C$ drastically reduced the open circuit voltage. Zäll et al., (2023) investigated the effectiveness of SiO_2 ARC with close pore structure and reported that the closed pore structure is well suited for tempered and arid climates with regards to humidity, temperature, and abrasion resistance. However, there is need of additional information with regard to the evaluation of optical and electrical properties of the solar cell with and without ARC.

In this study, we evaluated the effect of TiO_2 ARC and its thickness on reflectance, current density, open circuit voltage and efficiency of $GaAs$ solar cell with and without ARC. The work was carried out in COMSOL Multi-physics environment. The results would help the solar cells manufacturers in designing a solar module with effective ARC and higher efficiency.

METHODOLOGY

THEORETICAL BACKGROUND

The major field of this research involved optical and electrical theories. The optical theory comprised the concept of reflection of electromagnetic waves in the visible region while the electrical theory connected the electrical parameters such as current density, open circuit voltage, maximum power and efficiency of the solar cell.

Optical parameters

The destructive interference occurs between two reflected beams; front and rear surface which leads to the cancellation of beams thereby minimizing the unwanted reflection. The theoretical optimum refractive index of a single layer ARC is around 1.23 when it satisfies the relation in the equation (1).

$$n_{ARC} = \sqrt{n_0 \times n_s} \qquad (1)$$

where n_{ARC} is the ARC refractive index, n_0 is the refractive index of the air, and n_s is the refractive index of the substrate (solar cell)

However, it is difficult to source a material with such a natural refractive index (Mandong and Uzum, 2021). In this case the coating thickness can be optimize, so that the refractive index of the coating material would be reduce toward the optimum range. Equation (2) can be used to optimize the single-layer anti-reflection coating thickness based on the refractive index, wavelength and angle of incident.

$$d = {}^{\lambda}/_{4n_{ARC}} \qquad (2)$$

where d is the thickness of the ARC, and λ is the wavelength of the incident electromagnetic wave at visible region.

The optical path difference with regard to coating thickness and refractive index can be obtained by using equation (3). As the coating thickness and path difference are directly proportional (Tian, Li and Wu, 2017), thus fabricating the ARC remains the challenge during experimental deposition of the coating due to surface roughness at the heterogeneous interface of coating and the substrate (solar cell) as shown in Figure 1.

$$\theta = \frac{2\pi d n_{ARC}}{\lambda} \qquad (3)$$

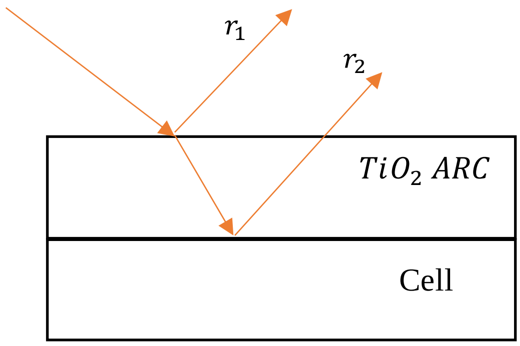

Figure1: Interference of light through the coating and substrate layer (Mandong and Uzum, 2021)

The resultant reflectivity between the coating and solar cell can be evaluated as:

$$R = |r_2| = \frac{r_1{}^2 + r_2{}^2 + 2r_1 r_2 \cos 2\theta}{1 + r_1{}^2 r_2{}^2 + 2r_1 r_2 \cos 2\theta} \qquad (4)$$

where the reflection from the coating is r_1, r_2 is the reflection from the substrate (solar cell) and θ is optical path angle.

Electrical Parameters

When photons are absorbed by the solar cell, it excite the electron from the valence band to the conduction band (Muhammad *et al.*, 2019). This would create holes and electrons movement at the deflation region and cause the flow of electric current due to electric field that exist at the junction. The output current density can be calculated from the equivalent electric circuit of the single diode model using equation (5):

$$J = J_{Ph} - J_o exp\left(\frac{q(V+JR_s)}{nk_B T} - 1\right) - \frac{(V-JR_s)}{R_{sh}} \qquad (5)$$

where J is the output current density of the cells (mA/cm^2) , J_o is the diode saturation current density (mA/cm^2) which is the current that flows in the diode when large reverse voltage is applied, J_{Ph} is the photocurrent density (mA/cm^2) which depicts the amount of current generated in the cell when it is exposed to photon energy, R_s is the series resistance (Ω) due to the high sheet resistance and grid arrangement, R_{sh} is the shunt resistance (Ω) results from imperfection from the junction, k_B is the Boltzmann constant $(1.38 \times 10^{-23} J/K)$, q is the electric charge $(1.602 \times 10^{-19} C)$, V is the terminal or applied voltage (volt), n diode ideality factor which signifying the charge transport efficiency, T is the temperature (K) generated as a result of the absorption and generation process inside the cell and from the front surface.

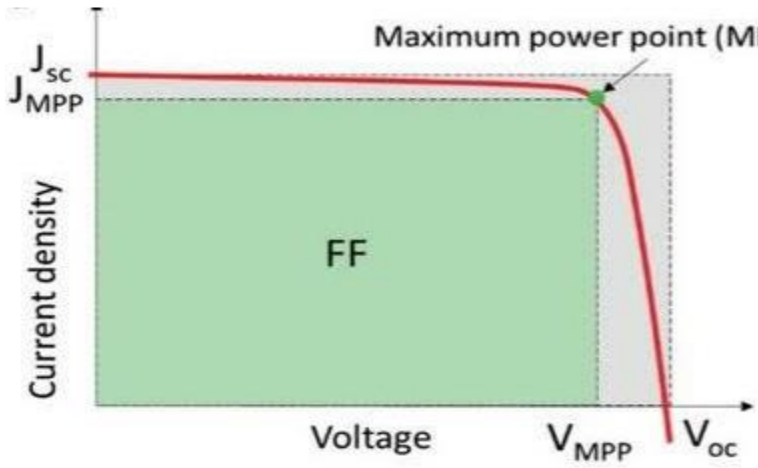

Figure 2: J-V curve of solar cells based on single-diode model (Muhammad *et al.*, 2019)

At zero terminal voltage that is ideal case, the photocurrent density is equivalent to short circuit current density J_{sc} which is the current that flows through the junction under illumination at zero applied voltage $(V_{app} = 0)$ as shown in Figure 1. Likewise, when the terminal current is zero $(J = 0)$, the open circuit voltage V_{oc} of the cell can be deduce from the J-V curve or calculated using equation (6):

$$V_{oc} = \frac{nK_BT}{q} \ln\left(\frac{J_{sc}}{J_o} + 1\right) \quad (6)$$

The power output or maximum power can also be deducing from the slope of J-V or calculated using equation (7) when the dimensionless fill factor (FF) (a measure of the deviation of real J-V characteristic from the ideal) is less than one.

$$P_{out} = FF \times J_{sc} \times V_{oc} \quad (7)$$

The overall efficiency (η) of the solar cell when illuminated with the power irradiance (P_{input}) can be determine as the ratio of the power out to the power input as expressed in equation (8).

$$\eta = \frac{P_{out}}{P_{input}} \times 100\% \quad (8)$$

Moreover, open circuit voltage is the function of temperature as shown in equation (6), this temperature is responsible in influencing the charge generation and recombination at the junction which can affect the amount of the voltage generated. Therefore, evaluation of the temperature effect on the electrical parameters specifically J_{sc}, V_{oc}c and efficiency is required. Generally, utilizing the capacity of COMSOL Multi-physic software, the reflection coefficient of the solar cell with and without ARC is evaluated using equation (4), while the current density, open circuit voltage, maximum power and efficiency were evaluated base on equation (5), (6), (7) and (8) respectively.

SIMULATION

COMSOL Multi-physics is a finite element analysis, solver, and simulation software package for various physics-based, engineering and scientific applications. It allows users to model and simulate coupled physical phenomena across multiple disciplines, such as structural mechanics, optics, heat transfer, fluid dynamics, electromagnetics, and acoustic, among others. In this work the optical and electrical properties are coupled and simulated using electromagnetic and semiconductor model.

Layers arrangement and Input Parameters

The two-dimensional structure were selected based on previous literature (Abu-Shamleh *et al.*, (2021);,Mbengue *et al.*, (2016);,Parajuli *et al.*, (2023)). As shown in figure 3, the height of the $GaAs$ solar cells (n and p type) and the surrounding air were set as 600 nm and 100 nm in length, respectively.

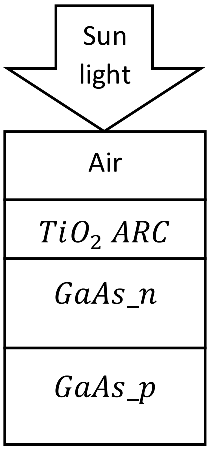

Figure 3: The diagram of $GaAs$ solar cell coated with TiO_2 ARC (Parajuli *et al.*, 2023)

In COMSOL multi-physics software, two modules were coupled, Electromagnetic Waves (Frequency domain), and Semiconductor module, so as to evaluate the optical and electrical properties. The Electromagnetic Waves module required the optical constants, illumination intensity and the perfect conductor's properties to calculate the total photo-generation, while the semiconductor module required the materials and electrical parameters which includes the trap assisted recombination and Shockley-Read-Hall (SRH) recombination. These modules use the photo-generation to solve the current-continuity equation as a result of coupling with Semiconductor and Electromagnetic wave modules. Most material properties for all domains were extracted from the COMSOL Multi-physics version 5.6 library as shown in table1.

Table 1: Material properties of $GaAs$ solar cells

Parameter	$GaAs$ $(n-type)$	$GaAs$ $(p-type)$
Relative permittivity	13.8	13.8
Band gap	$1.4V$	$1.4V$
Electron affinity	$4.2V$	$4.2V$
Effective density of state (Nc)	$1\times10^{16}cm^{-3}$	$3\times10^{18}cm^{-3}$
Effective density of state (Nv)	$1\times10^{16}cm^{-3}$	$3\times10^{18}cm^{-3}$
Electron mobility	$1100cm^2/Vs$	$1100cm^2/Vs$
Hole mobility	$300cm^2/Vs$	$300cm^2/Vs$
Electron lifetime	$100\mu s$	$100\mu s$
Hole lifetime	$100\mu s$	$100\mu s$
Temperature	$300K$	$300K$
Donor concentration	$9\times10^{19}cm^{-3}$	$1\times10^{21}cm^{-3}$
Light intensity	$0.1W/cm^2$	$0.1W/cm^2$

Models Set-up

During the simulation, boundary conditions for both Electromagnetic Wave, Frequency Domain Model (ewfd) and Semiconductor model were appropriately defined. For Electromagnetic Wave, Frequency Domain Model, a periodic boundary conditions were assigned at the two-vertical layer of the $GaAs$ solar cell. However, the ARC layer was set to be a perfectly matched layer in order to present artificially absorbing boundaries and prevent unwanted field reflections and scattering. To implement the electromagnetic field source, the periodic ports were assigned at the upper and bottom boundaries of the air and substrate domains. The wave excitation slit port in the air domain is activated so as to serve as an initial source of an incidence power irradiance at an angle of 70^0.

The dimension of all layers remains constant except for the cubic anti-reflection coating layer where it optimized at different coating thickness of 10nm to140nm in length. The materials of every layers (domain) were inserted from the COMSOL library as done by (Abu-Shamleh, Alzubi and Alajlouni, 2021). For the accuracy of the result, the free triangular finer mesh was selected and refine at different size of each domain due to edge angle. To avoid inconsistences in computed results and hardware, the error bound was set as 0.5 under adaptation and estimation error.

The total photo-generation were computed from wavelength domain so as the percentage reflectance of the cell can be evaluated with and without coating. The semiconductor model used the computed total photo-generation obtain from electromagnetic wave, frequency domain model and evaluate the electric field and electric potential, hole and electric concentration of the solar cell. Therefore, the current and voltage curved (J-V) can be characterized which helps in calculating the fill factor, maximum power and overall efficiency of the solar cells using global evaluation. The effect of operating temperature on the electrical parameters were evaluated by varying the range of the temperature from $25℃ - 70℃$.

RESULTS AND DISCUSSION

The effects of ARC and its thickness on reflectance and current density as well as effect of temperature on the open circuit voltage and current density of the cell with ARC are evaluated.

Reflectance of solar cell with and without ARC

The input power irradiance used as the plane wave (400-800nm) was A.M1.5 solar spectrum (Zandi *et al.*, 2020). The percentage reflection of the cells without coating was found to be 32% when the solar irradiance was applied. However, when the solar cell coated with TiO_2 ARC at thickness of 80nm and an angle incidence of 70^0, the reflection was reduced to 5% at the broad range of wavelength (680nm-720nm) as shown in figure 4. This result revealed the intercept stability between TiO_2 ARC and $GaAs$ solar cell as a substrate where light can destructively interfere.

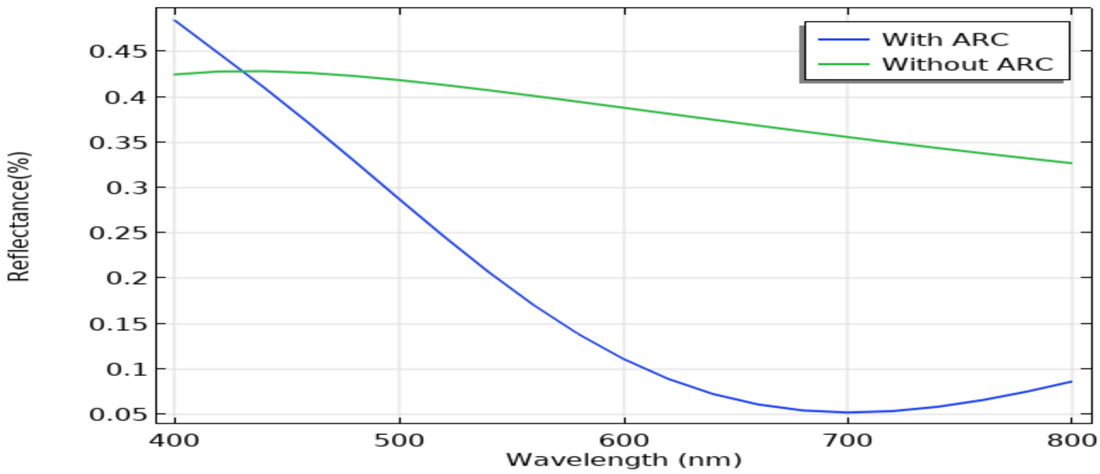

Figure 4: Reflectance of $GaAs$ solar cell with and without TiO_2 ARC

Effect of ARC thickness on reflectance

Despite the ability of the ARC in reducing the front surface reflection, optimization of the ARC thickness is required to achieve the optimum thickness that would significantly decrease the reflection lost in solar cell.

Looking at the figure 5, it observed that the coating thickness directly affect the reflectivity of the light, where an increase in coating thickness leads the reflectivity of the light to increase by scattering the incident light and vise visa. This would either reduce or improve the amount of transmitted and absorbed photons by the solar cell. Therefore, archiving the optimum coating thickness depends on the complete structure of the solar cells starting from the top layer up to the bottom layer of the solar cells. As such it shows that, 80nm is the desired ARC thickness that improve the absorption capacity of the solar cell.

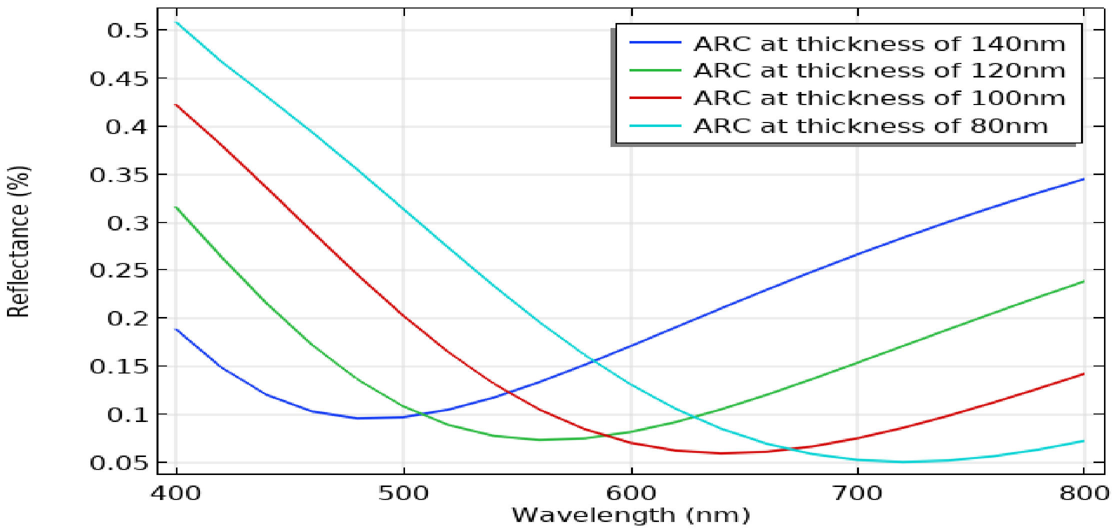

Figure 5: Reflectance of $GaAs$ solar cell with TiO_2 ARC at different thickness

Influence of ARC on Electrical J_{sc}, V_{oc} and Efficiency

Solar cells use photon to generate electricity depending on their energy band gap. Therefore, high transmission and absorption of photons that can generate the electric field at a junction is required. Having the higher absorption can positively affect electrical parameters such as current density, open circuit voltage, maximum power, fill factor and efficiency. As shown in table2, the short circuit current density, open circuit voltage, maximum power and overall efficiency of the solar cell were increased when coated with TiO_2 ARC. These results relatively have shown an improvement when compared to the work of (Parajuli *et al.*, 2023).

Table 2: Electrical and optical values of $GaAs$ solar cell with and without TiO_2 ARC

Parameter	Reflectance (%)	$J_{sc}(mA/cm^2)$	$V_{oc}(V)$	$P_{max}(W)$	FF (%)	Efficiency (%)
Without ARC	32	3573.1	0.82	190.15	65	19
With ARC	5	5001.1	1.03	254.92	50	25

In comparison, figure 6 shows the J-V curved of the solar cell with and without TiO_2 ARC at 27℃ and thickness of 80nm. The result indicates an improvement in both the current density and open circuit voltage.

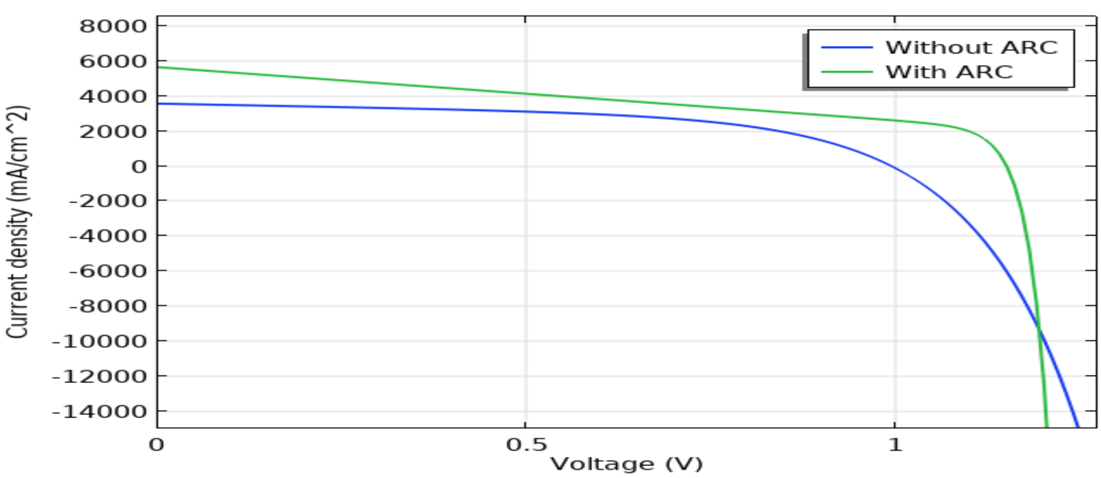

Figure 6: J-V Curved of $GaAs$ solar cell with and without TiO_2 ARC

Variation of temperature with J_{sc} and V_{oc}

Majority of the incident photons are not converted to electricity when falls on solar cells, but some are lost as a result of heat generation within the solar cells (Nishioka, Moe and Ota, 2019). This heat is generated as a result of recombination and absorption processes which later rise the temperature of the cells. From the result obtain, as the temperature varied at the range of 25℃ – 70℃ at the interval of 10℃ as shown in figure 7, the rise in operating temperature of the coated solar cell decreases the open circuit voltage from 1.030 to 1.015V while the short circuit current negligibly increased. Moreover, when the temperature is raised to 70℃, the overall efficiency of the coated solar cell reduced from 25% to 23%.

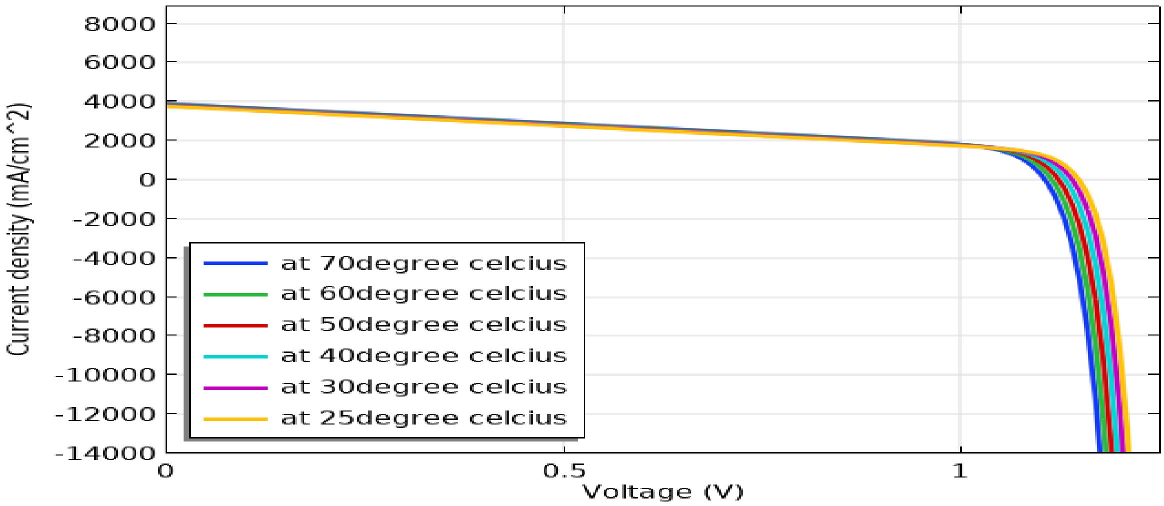

Figure 7: Variation of temperature with J_{sc} and V_{oc}

Despite the high temperature effects on solar cell but the efficiency is only reduced to 2%. This revealed the effectiveness of TiO_2 as ARC material compere to the others.

CONCLUSION

We found that, the Titanium dioxide (TiO_2) Antireflection Coating (ARC) enhanced the solar cell efficiency from 19% to 25%. This increase was due to the increase in the total reflectance from 32% to 5%. This result revealed a very good development, since the overall efficiency of the solar system that employing photovoltaic panels with ARC will definitely encourage the use of renewable energy sources. On the other hand, increase in the absorption of photons by the solar cell and the process of current generation within the cells led to rise in operating temperature. When the temperature raised to 70℃ the open circuit voltage decreases from 1.030V to 1.015 which reduced the efficiency 23%. Thus, this decrease in open circuit voltage can be conceded to get efficiency improvement of 6%.

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