International Research Journal of Innovations in Engineering and Technology (IRJIET)

ISSN (online): 2581-3048
Volume 6, Issue 11, pp 124-129, November-2022
https://doi.org/10.47001/IRJIET/2022.611017

Studying the Effect of Variable Temperatures on the Output of a Perovskite Solar Cell (ZnTe /$CH_3NH_3PbI_3/TiO_2$/ZnO/FTO) Using SCAPS-1D Software

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***Abstract* - The program SCAPS-1D was used to simulate the solar cell adopted in this research, and it was a starting point as a conventional perovskite solar cell (ZnTe/$CH_3NH_3PbI_3/TiO_2$/ZnO/FTO), as the thickness of the absorption layer p-$CH_3NH_3PbI_3$is 1 µm and thickness of windows layer n-ZnO is 0.1 µm and buffer layer $TiO_2$of thickness of 0.05 µm, which is used as a layer that prevents forward contact process or Front leakage for minority carriers (gaps), this leakage is undesirable because it is an insulating and chemically active layer with different operating temperatures ranging between (270K-320K), also the thickness of transparent conduction oxide layer (FTO) is 0.1µm. In this paper, the effective temperature on the outputs of the solar cell was studied as well as its effect on the quantum efficiency QE and current-voltage curve (I-V). The optimum available of this perovskite ($CH_3NH_3PbI_3$) solar cell results at 300K as follows: [V_{oc}=1.288(V), J_{sc}=25.04mA/cm^2,FF=89.54%,η=28.88 %].**

Keywords: SCAPS-1D; perovskite $CH_3NH_3PbI_3$solar cells; (I-V) curve.

I. INTRODUCTION

The perovskite solar cells are photovoltaic devices that convert electromagnetic radiation (light, infrared, ultraviolet rays) coming from sun into usable electrical energy[1].

The ternary semiconductors as perovskite were still interested to researchers because most of them have direct energy gaps extending from ultraviolet region to infrared region and their adaptation to different impurities. Solar cells based on perovskite are the biggest candidate and competitor to the rest of the other conventional solar cells because of their high efficiency, and it is a strong competitor to polycrystalline silicon, which is still dominant in the photovoltaic energy market that is currently used in markets[2]. The general formula for perovskite is ABX3, where A and B are two positive ions, so that the ion (A) is greater than the ion (B) and the ion (X) is a negative ion that binds between the oxides or halides, figure (1) shows the crystal structure of perovskite[2].

The perovskite is characterized by great dielectric constant, long life and high efficiency for absorbing the solar light. The halide in the molecule from organic halides or non organic halides as tin or lead has been found through recent researchers that the charges of perovskite compounds exist in the form of free electrons and holes because their binding energy is low enough to separate charges at room temperature [3].

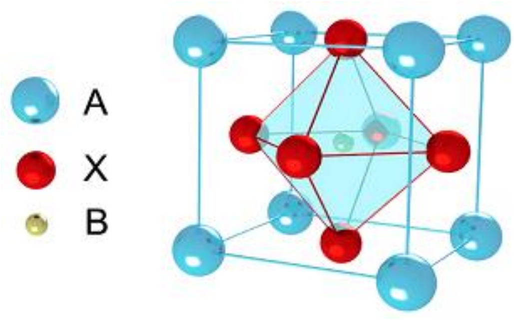

Figure 1: The crystalline structure of perovskiteABX_3

The absorption perovskite layer ($CH_3NH_3PbI_3$) is located between two layers that conduct electrons and holes is connected to transparent layer to allow sun radiation to pass through it. The perovskite cell is one of the best environmentally friendly solar cells and also its properties have highly efficiency compared to the rest of the other conventional solar cells [4].

Several researchers added a back reflection layer on the solar cell and studied the effect of this layer on the current-voltage (I-V) curve.

In 2014, Bernal, Yang investigated the properties of a perovskite solar cell made of tin and replaced it with halides such as bromine or iodine to facilitate charge transfer to the ETL layer, as well as to prove that the organic part of perovskite does not contribute In the process of energy production [5]

In 2017, Farhana Anwar and his group investigated the effect of gap transport layer (HTL) of different materials on

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the perovskite solar cell and to obtain good cell performance using simulation software SCAPS 1-D for compound ($CH_3NH_3PbI_3$) and achieving an efficiency 20.23% for the transport gap layer (HTL) which is (CU_2O) [6].

In the year 2019, Ismaila T-Rello and his group investigated the effect of the transport gap layer (HTL) on working of the perovskite cell and used simulation program SCAPC 1-D and compared the results in the presence of a layer (HTL). And in the absence of it, he recorded the thickness of the absorption layer between (50-500)nm, and it was found during the study that the greater thickness of the absorption layer, the higher efficiency of the solar cell based on the transfer gaps layer (HTL), so that the efficiency of the conversion reached to 20.56% and the efficiency was in the absence of layer (HTL) is reached to 15.53% [7].

In 2020, the researcher Sani Faruk conducted to study on alternative compounds for lead-based perovskite cells, and he found that tin metal ranked first, where the efficiency is 24.28%, and also concluded that Halides can be exchanged to obtain good energy gap [8].

In this paper, the effect of changing temperatures on the properties of the curve (I-V) and Quantitative efficiency (QE) as well as the outputs cell which are voltage open circuit (Voc), current short circuit (Jsc), fill factor (FF) and the efficiency conversion (η) was studied, for the solar cell ($CH_3NH_3PbI_3/TiO_2$/ZnO/FTO) after adding back reflection layer (BSF) ZnTe as for cell that works to reduce re-adhesion at the back contact and reduce the thickness of the absorption layer which is characterized by having a wide energy gap [9]. Where the effect of different temperatures from (270-400) K was studied.

II. MATERIALS AND RESEARCH METHODS

Digital simulation of solar cells devices has proven over years to be an effective tool for studying and understanding many of physical properties for complex solar cells devices. Computer simulation is a technique for studying and analyzing the behavior of real device or an imaginary system by imitating it by using a computer application system [10]. Thus, it helps to reduced the processing costs and time spent in manufacturing solar cells by providing useful information on how to change production parameters to improve device performance.

The SCAPS-1D program was used to simulate on one-dimensional solar cell, and the user could describe a solar cell consisting of a maximum seven layers with different characteristics. The SCAPS-1D simulation program solves basic one-dimensional semiconductor equations such as the Continuity equation, Poisson's equation, and carrier density (electrons and holes) caused by difference in the concentrations of charge carriers and recombination, and these equations as follows:

$$jn = q\mu n\, n\varepsilon + qDn\frac{dn}{dx} = q\mu n(n\varepsilon + \frac{KT}{q}\frac{dn}{dx}) = nn\frac{dEFn}{dx} \quad \cdots\cdots\cdots(1)$$

$$jn = q\mu p\, P\varepsilon + qDn\frac{dn}{dx} = q\mu p(p\varepsilon + \frac{KT}{q}\frac{dn}{dx}) = \mu pP\frac{dEFp}{dx} \quad \cdots\cdots\cdots(2)$$

Where ε: Electric Field, μn-μp: mobility of electron-hole, Jn-Jp: current density of electron-hole.

The continuity equation for the electron can be written as

$$\frac{\partial n(x)}{\partial t} = Gn(x) - Rn(x) \quad \cdots\cdots\cdots(3)$$

$Gn(x)$:generation process of electron.

$Rn(x)$: recombination process and continuity equation for holes.

$$\frac{\partial p(x)}{\partial t} = Gp(x) - Rp(x) \quad \cdots\cdots\cdots(4)$$

$Gp(x)$: generation process of holes.
$Rp(x)$: recombination process of holes.

As for the poisson's equation, it links between the charge density equation and the electron voltage (electrostatic potential Φ), which is the starting point for obtaining a qualitative solution to the variables in the static electricity of semiconductors [11].

$$\frac{d\ln(E(x))}{\partial x} \cdot \frac{d\phi(x)}{dx} + \frac{d^2\phi}{dx^2} = \frac{f(x)}{\varepsilon(x)} \quad \cdots\cdots\cdots(5)$$

If ε helds as a constant, the poisson's equation is in the following form:

$$\frac{d^2\phi}{dx^2} = -\frac{f(x)}{\varepsilon} \quad \cdots\cdots\cdots(6)$$

The current that passes through the solar cell can be calculated using the equation:

$$I = I_o\,(\exp\frac{qv}{KT} - 1) \quad \cdots\cdots\cdots(7)$$

Where I is the load current, I_o represents the reverse saturation current, Trepresents the temperature and K represents the Boltzmann constant, open circuit voltage Voc can be calculated from the following relationship:

$$Voc = \frac{KT}{q}\ln\frac{Isc}{Io} + 1 \quad \cdots\cdots\cdots(8)$$

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Fill factor can be defined as the square of the curve (I-V) and it's amount is mainly related to the loss resistance of the solar cell [12], and can be calculated from the following relationship:

$$FF = \frac{Vm\,\mathrm{Im}}{Voc\;Isc} \qquad \cdots\cdots\cdots(9)$$

Where I_m V_m represents maximum current and voltage density generated by the solar cell.

The efficiency of the solar cell is also calculated from the relationship:

$$\eta = \frac{output\ Power\,(Pout)}{Input\ Power\,(Pin)} \times 100\% \qquad \cdots\cdots\cdots(10)$$

The efficiency equation can be written in another way:

$$\eta = \frac{FF \times Isc \times Vos}{Pin} \times 100\% \qquad \cdots\cdots\cdots(11)$$

Figure (2) shows the interface in the SCAPS-1D program of the perovskite solar cell adopted in this paper.

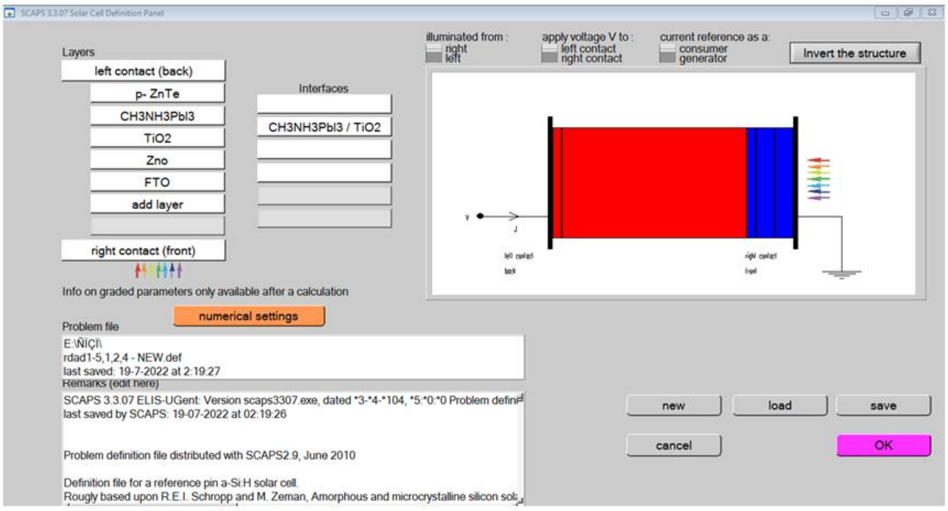

Figure 2: SCAPS-1D program interface for the cell used

Table 1: parameters of the Perovskite solar cell layer

Parameters	p-ZnTe	$CH_3NH_3PbI_3$	TiO_2	ZnO	FTO
Thickness (µm)	0.05	1.0	0.05	0.1	0.1
Band gap (eV)	2.25	1.55	3.2	3.3	4.2
Electron affinity (eV)	3.65	3.9	4.9	4.4	4.5
Dielectric permittivity (relative)	14	6.5	9	9	10
CB. effective density of states ($1/cm^3$)	7.50E+17	2.2E+18	1.00E+21	2.20E+18	1.20E+20
V.B. effective density of states ($1/cm^3$)	1.5E+19	1.8E+19	2.00E+20	1.80E+19	7.80E+20
Electron thermal velocity (cm/s)	1.000E+7	1.00E+7	1.000E+7	1.000E+7	1.00E+7
Hole thermal velocity (cm/s)	1.000E+7	1.00E+7	1.000E+7	1.000E+7	1.00E+7
Electron Mobility (cm^2/Vs)	70	2	2.00E2	100	20
Hole Mobility (cm^2/Vs)	50	2	1.0E2	25	100
Shallow uniform donor density, N_D ($1/cm^3$)	0	0	1.00E+19	1.00E+19	1.00E+19
Shallow uniform acceptor density N_A ($1/cm^3$)	1.00E+19	1.00E15	0	0	0
Defect type	Single Acceptor	Single Donor	Single Donor	Single Donor	Single Donor
Capture Cross Section Electrons (cm^2)	1.00E-12	1.00E-17	1.00E-15	1.00E-15	1.00E-15
Capture Cross Section Hole (cm^2)	1.00E-15	1.00E-12	1.00E-15	1.00E-12	1.00E-12
Nt ($1/cm^3$)	2.00E+14	1.00E+12	1.00E+13	1.00E+15	1.00E+15

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Table 2: Interface Parameters

Parameters	
Defect type	Neutral
Capture Cross Section Electrons (cm^2)	1×10^{-19}
Capture Cross Section Hole (cm^2)	1×10^{-19}
Nt (1/cm^3)	$1 \times 10^{+10}$

Effect of Temperature on (I-V) properties:

The temperature at which duo works affects its electrical properties, and the main reason for this is due to increase of minority charge carriers due to the (electron-hole) pairs, which results from the acquisition of an electron from valence band with sufficient energy, so it jumps to the conduction band leaving a hole in its place[13]. One of the negative consequences of high temperature increasing in the leakage current or saturation resulting from the minority carriers. The high temperature increasing the saturation current (Is) and reduces the barrier voltage due to the high leakage current, and the high temperature leads to decreasing in the value of the energy band gap [14].

When the value of the energy band gap decreased, the value of the current density increased, and the reason is that many incident photons will have enough energy to generate (electron-hole) when the energy of the energy band gap is much less than the energy of the photons and affect the electrical properties and the main reason for this due to the increasing the minority of charge carriers [15]. The temperatures effected on the saturation current [16] because the carrier density are exponentially related to the resulting temperature due to the electrons in valence band in which gained enough energy to move to conduction band, leaving hole in its place, thus reducing the barrier voltage and decreasing the width of the depletion region, the saturation current produced by increasing the minority carriers as shown in Figure (3).

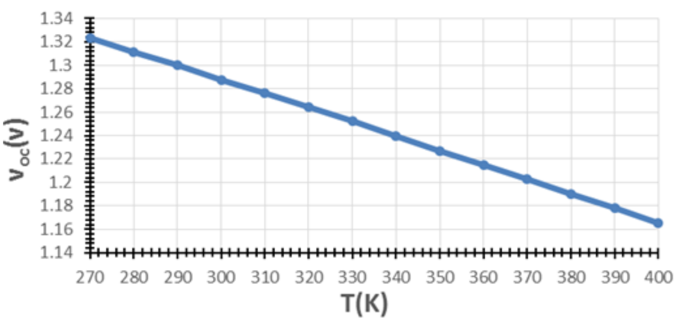

Figure 3: The influence of temperatures on the open circuit voltage Voc

When studying the effect of temperatures, we noticed decreasing in the value of the open circuit voltage (Voc) with increasing in temperatures, and the reason for this is that increasing in working point temperature to reduce the energy band gap, which increasing the heat of saturation current [13] , where it becomes more obvious with the increasing in temperatures, so the open circuit voltage decreasing with increasing in temperature due to the high saturation current [17] as shown in Figure (4), and the solar cell is considered good as it approaches Fill Factor of one, i.e. the closer shape of the curve current-voltage (I-V) to the square shape.

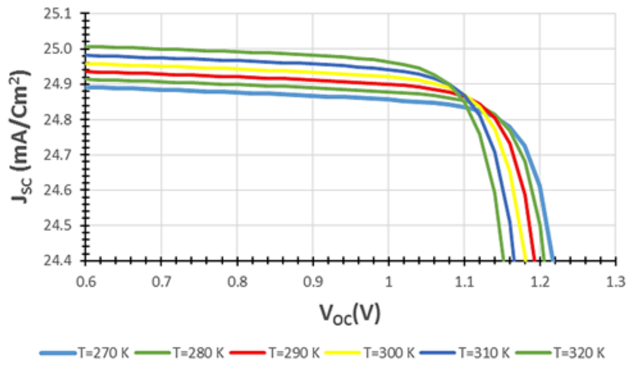

Figure 4: The influence of temperatures on the characteristic curve (I-V)

When temperatures raised, the Fill Factor decreases as shown in Figure (5), the reason for this is due to rising in diffusion current at the expense of the current density of the carriers and decreasing in the value of the open circuit voltage, which increased the connection of interface, which reducing the output of solar cell [18], and thus decreasing Fill Factor (FF).

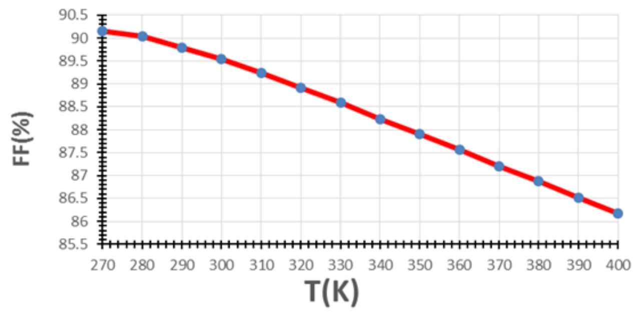

Figure 5: The influence of temperatures on the Fill Factor FF%

As for the short-circuit current (Jsc)does not depend to a large extent on temperatures, as the current increased slightly when temperature is increased, this is due to increasing in the absorption of the incident light as a result of decreasing in energy band gap resulting from increasing in temperatures [19] as in Figure (6).

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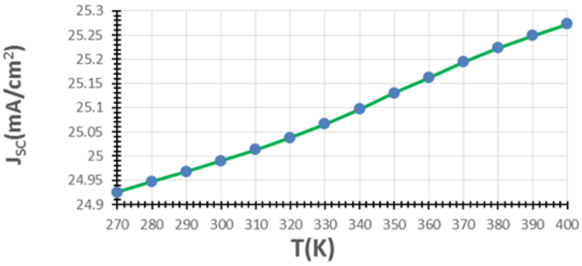

Figure 6: The influence of temperatures on short circuit current Jsc

When studying each of the above properties it is necessary to measure the efficiency of solar cell (η), one of the most important properties that researchers seek to improve in order to increasing yield of the solar cell at the lowest prices[15], the reason is that increasing in temperatures increased the heat leakage current (Is), which leads to a decreasing in (Voc), thus a decreasing in the efficiency of solar cell, as shown in Figure (7).

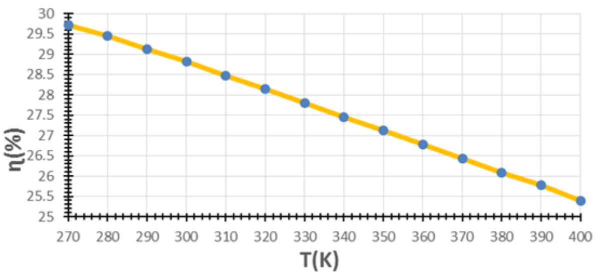

Figure 7: The influence of temperatures on the efficiency η

As for the effect of temperature on the Quantitative Efficiency (QE), its effect is very small, as shown in Figure (8), shows the effect of temperatures on the Quantitative Efficiency (QE), because the short-circuit current (Jsc) is slightly affected with increasing temperatures, while the open circuit voltage (Voc) decreased with increasing temperatures, due to increasing in saturation current due to decreased in the energy band gap since the density of charge carriers will be exponentially proportional to height temperatures. Thus, the effect of temperature on the quantitative efficiency (Q.E) will be very weak.

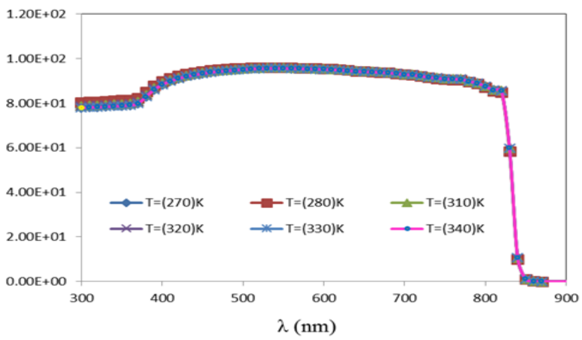

Figure 8: The influence of temperatures on the Quantitative Efficiency (QE)

III. CONCLUSION

When studying the effect of temperature, we noticed decreasing in the value of the open circuit voltage (Voc) with the increasing in temperatures. Minority carriers also when raising the temperatures, it was found that Fill Factor decreased, and it was found during this paper that the increasing in temperatures has an opposite effect contrary to what is expected, that is the increasing in temperatures reduced the efficiency of the solar cell. As for effect of temperatures on the Quantitative Efficiency (QE) has very little effect.

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Citation of this Article:

Raddad Salem Mahmoud, Raad A. Rassol, “Studying the Effect of Variable Temperatures on the Output of a Perovskite Solar Cell (ZnTe /$CH_3NH_3PbI_3$/TiO_2/ZnO/FTO) Using SCAPS-1D Software”, Published in *International Research Journal of Innovations in Engineering and Technology - IRJIET*, Volume 6, Issue 11, pp 124-129, November 2022. Article DOI https://doi.org/10.47001/IRJIET/2022.611017

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