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THE EFFECT OF TEMPERATURE DEPENDENCE ON TIN PEROVSKITE SOLAR CELL USING SCAPS 1D

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ABSTRACT

Perovskite solar cell (PSC) has become a force to reckon with in the renewable energy community because of its performance and low cost of production. Solar energy is one of the most demanding renewable sources of electricity. Electricity production using photovoltaic technology, not only helps meet the growing demand for energy, but also contributes to mitigate global climate change by reducing dependence on fossil fuels. Simulation is based on a mathematical design that describes the system. Numerical simulation technique of solar cells devices has over the years proven to be a viable tool for observing and understanding the properties of solar cell devices such as the optical, electrical and mechanical properties of complex solar cell devices. It also helps to reduce processing cost and time spent on solar cell device fabrication by providing useful information on how to vary the production parameters to improve the device performance. Solar cell capacitance simulator in one dimension (SCAPS-1D) was used in the modeling and simulation of sandwiched perovskite solar cells (PSCs) with a planar hetero-junction structure in the arrangement of the sandwiched model (FTO/CdS/$CH_3NH_3SnI_3$/HTM). The energy band diagram, I-V characteristics and other parameters was obtained. The configuration for better performance was then determined, from which further simulations were carried out. When the operating temperature was varied the result shows an overall efficiency of 24.25%, FF of 82.80%, J_{SC} of 30.73mA/cm^2, V_{OC} of 0.95V was obtained.

Keywords: Perovskite Solar Cell, numerical simulation, SCAPS, conversion efficiency, ETM

INTRODUCTION

In studying, Perovskite solar cell, the new generation of photovoltaic is expected to replace the old types of solar cells. Perovskite solar cell (PSCs) as a promising candidate is abundant in nature which offers low cost, stability and high energy conversion efficiency (Anish et al., 2016). Perovskite solar cell has excellent features such as long carrier, diffusion lengths and widely tunable with great light absorption potential. More especially, perovskite solar cell is a perovskite structured compound, most commonly a hybrid organic-inorganic lead or tin halide-based material as the light-harvesting active layer, cheap to produce and simple to manufacture. The absorber material is the heart of the solar cell which forms a junction between the electron transporting material and hole transporting material called an interface. It is a type of solar cell which includes a perovskite structured compound called hybrid organic-inorganic lead or tin halide-based material, as the light harvesting active layer which is a p type doping concentration (Balema, 2009). Also, it has the potential of achieving higher efficiencies and commercially attractive at very low production cost. The common once is methyl ammonium lead tri iodide ($CH_3NH_3PbI_3$) and methyl ammonium tin tri iodide ($CH_3NH_3SnI_3$) while others are methyl ammonium chlorine tri iodide ($CH_3NH_3ClI_3$) and methyl ammonium bromine tri iodide ($CH_3NH_3BrI_3$). Tin based perovskite solar cell serves as an alternative to lead because it is nontoxic, its visible absorption spectrum is wider than that of lead, it has a narrow bandgap of about 1.3eV and its efficiency is rapidly from 6.4% to 19.3% (Du *et al.*, 2006). Researchers have made several efforts in contributing to the development of perovskite semiconducting materials simulation which has led to the rise of low cost and high efficiency with respect to simulation of the solar cell capacitance simulator-one dimension (SCAPS) but not much has been done on simulation of tin perovskite in this category of photovoltaic cells in particular and solar cells generally.

Numerical simulation of tin based perovskite solar cell: effects of absorber parameters and hole transport materials by Aditi Toshniwal in 2017 revealed how the thickness (350-500nm) and defect density of the absorber material strongly influence the PCE of the device and various types of hole transporting material such as spiro-OMeTAD, Cu_2O, copper thiocyanate (CuSCN) and poly (3-hexylthiophene-2,5-diyl) (P3HT) where compared and analyzed to improve the performance of the solar cell. He further said that an HTM needs high carrier mobility and should form a defect free interface with the absorbing layer to minimize carrier recombination (Aditi *et al.*, 2017).

Hossain and co-workers built a simulation based on PSCs with ZnO as the ETM layer by using SCAPS. They showed that the device with ZnO as the ETM layer can obtain a high efficiency of 22.83% compared with TiO_2 as the ETM layer (Hossain *et al.*, 2015).

According to Hui-Jing Du in 2016, talks about the device simulation of lead-free $CH_3NH_3SnI_3$ perovskite solar cells with high efficiency. He found out that during simulation, the solar cell performance can be improved to some extend by adjusting the doping concentration of the perovskite absorption layer and the electron affinity of the buffer and HTM, while the reduction of the defect density of the perovskite absorption layer significantly improves the cell performance. By further optimizing, they obtained results of the PCE to be 23.36%, J_{SC} of 31.59mA/cm^2, V_{OC} of 0.92V and FF of 79.99% (Du *et al.*, 2006).

A Comparative Study of Different ETMs in Perovskite Solar Cell with Inorganic Copper Iodide as HTM was carried out indicating Lead-based perovskite solar cell ($CH_3NH_3PbI_3$) (PSC) with CuI as HTM, TCO, IDL and different ETMs (TiO_2, CdS, ZnSe, ZnO, ZnOS) are studied by SCAPS Simulation which shows that CuI as alternate HTM has the potential to be used with perovskite absorber and can replace the Spiro-OMETAD which is expensive and suffers from degradation. The highest PCE achieved is 23.47%. The thickness of the layers has a great influence on the performance parameters of the solar cells. After optimizing the thickness of all the layers, we get a PCE of 26.11%. (Salah *et al.*, 2018).

In addition, the thickness of absorber layer was changed from 0.1µm to 0.8µm, the good performance of a device is achieved at the thickness of 0.6 µm hence the thickness of the absorber layer is set at 0.6µm. design and simulation of high efficiency tin halide perovskite solar cell came up with the fact that by decreasing the defects in the absorber layer and improving the material quality, the device performance will be increased and the minimum defect density for the good efficiency was 10x14cm^{-3}. The suitable band gap for the good absorption and to reach higher performance is predicted as 1.3eV. The operating temperature was changed from 300K to 450K to observe the changes in the PV parameters of the device. The simulation demonstrates that the $CH_3NH_3SnI_3$, attain a PCE of 24.82%. (Usha *et al.,* 2017). Many works have been reviewed from the related literatures but none of the authors have discuss the effect of temperature dependence on tin perovskite solar cell using SCAPS 1D which is the gap that this study seeks and will be contributed to knowledge.

SCAPS was chosen over other numerical simulations programme such as SETFOS, AFORSHET and AMPS-1D because SCAPS is cheap, saves time and energy, it has variety of properties related with solar cells such as energy bands concentration, current-voltage characteristics, capacitance-voltage characteristics, capacitance-frequency characteristics and quantum efficiency characteristics and also it has a very intuitive operation window and diversified models which is used for grading, defects and recombination.

The working condition in SCAPS shows that change in operating temperature and illumination has affected the performance of solar cells due to change in carrier concentrations, mobility of the charge carriers, resistance and band gap of the materials. The role of temperature in the simulation studies and fabrications is 300K which is chosen as the operating temperature. In a given place the operating temperature varies with latitude, altitude, day of the year and time of the day. In this work, temperature was varied between 270K and 600K to determine the actual behavior of perovskite based solar cells.

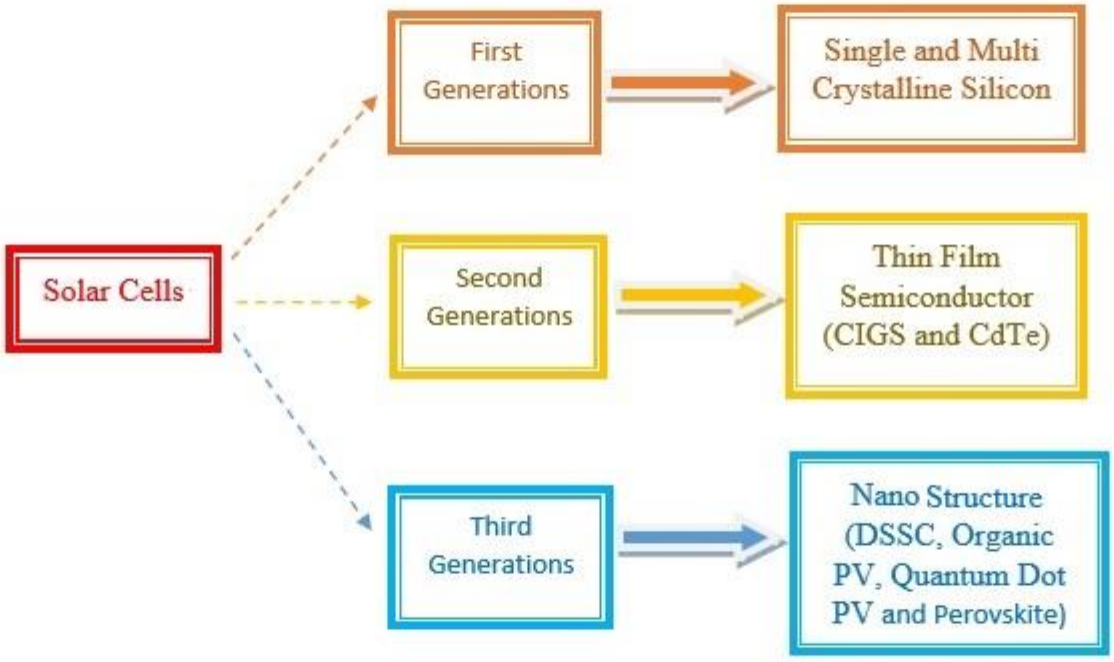

Figure 1: Solar cells generation technology (Usha *et al.*, 2017)

MATERIALS AND METHODS

Figure 2 shows the proposed model for tin based perovskite solar cell (Huang *et al.,* 2016). The performance of tin based perovskite structure is determined by varying the operating temperature between 270K and 600K and measuring the associated parameters. FTO is taken as the front contact material and Ag is taken as the rare contact material.

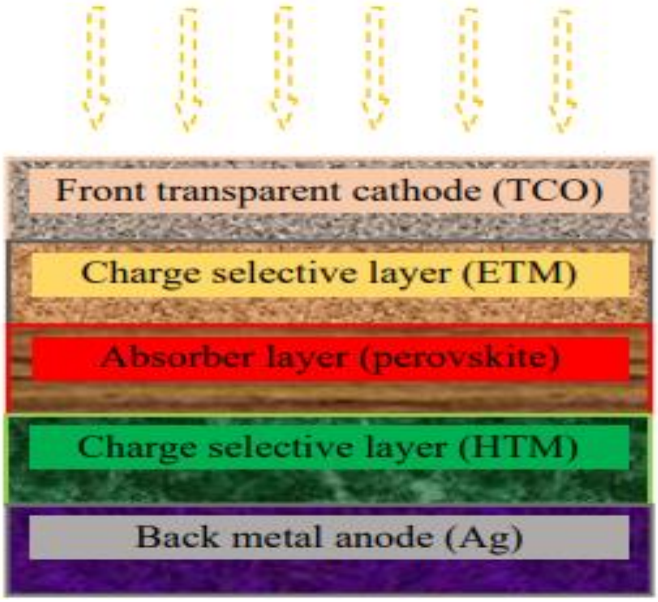

Figure 2: Layers of perovskite structure (Minemoto *et al.,* 2014)

SCAPS-1D is a one-dimensional solar cell simulation program based on three coupled differential equations by solving the basic semiconductor equations such as Poisson equation, continuity of electrons and holes (Bube, 1998 Burgelman *et al.,* 2000). SCAPS analyses the physics model in PSCs and it explains recombination profiles, electric field distribution, carrier transport mechanism and individual current densities. Five equations are combined to explain transport in semiconductors which are drift and diffusion current density equation for both electrons and holes, electric field equation which is related to Poisson equation and continuity equation for both electrons and holes. The essence of these five equations is aimed at knowing the quantity of current that is coming out of the solar cell device and can be solved numerically based on some assumptions. These five equations can be used to explain SCAPS based on

$\eta_{total} = \eta_{absorption}$ x $\eta_{excitation}$ x $\eta_{drift/diffusion}$ x $\eta_{separation}$ x $\eta_{collection}$

Drift and Diffusion Current Density for Electrons and Holes

Drift is charged-particle motion in response to an electric field. In an electric field the force acts on the charged particles in a semiconductor, which accelerates the positively charged holes in the direction of the electric field and the negatively charged electrons in the direction opposite to the electric field. Diffusion is a process by which particles tend to spread out from regions of high particle concentration into regions of low particle concentration as a result of random thermal motion. The driving force of diffusion is a gradient in the particle concentration. In contrast to the drift transport mechanism, the particles need not be charged to be involved in the diffusion process.

From equation 1 and 2 shows that whenever drift current occurs, there will be presence of electric field due to large electric field result to dominant of drift current and if diffusion occurs, there will be presence of concentration gradient due to small electric field result to dominant of diffusion current. As a charge carrier is moving from one semiconductor type to another, it will change the charge balance in the space charge region (SCR), which becomes depleted of free charge carriers. The new charge balances in the SCR, cause an electrical field from the n-type (positively charged donor defects) to the p-type (negatively charged acceptor defects) semiconductor. In the field, free charge carriers will be promoted as a result of drifting in one direction, and opposed in the other direction, depending on the rate of their charge. Thus, there are two competing forces in the p-n junction, diffusion opposed by drift.

$I = neAV_d$

$I/A = neV_d$

Where I/A = J which is represented as current density flowing for both electron and hole, n = density of charge carriers, e = charge carriers is the same for both electrons and holes having opposite sign, (drift velocity) $V_d = \mu\mathcal{E}$: μ = mobility of charge carriers, Ɛ = electric field across the semiconductor material

$$J_e = q\mu_n n\mathcal{E} + qDe\,\frac{dn}{dX} \qquad (1)$$

$$J_P = q\mu_p P\mathcal{E} - qDp\,\frac{dP}{dX} \qquad (2)$$

Electron and hole mobility μare the parameter that characterizes transport due to drift. Although the electrons move in the opposite direction to the electric field, the number of collisions increases which decreases the mobility. Increasing the temperature increases the collision rate of charged carriers with the vibrating lattice atoms, which results to low mobility. Where J_e is the electron current density, q is the charge, n is the electron, E is the electric field, De is the electron diffusion, $\frac{dn}{dX}$ is the concentration gradient of electron in one dimension, J_P is the hole current density, p is the hole, x is the distant in x direction, Dp is the hole diffusion, $\frac{dp}{dX}$ is the concentration gradient of hole in one dimension, $q\mu_n n\mathcal{E}$ is the drift and $qDe\frac{dn}{dX}$ is the diffusion.

In addition, if a piece of p-type material is placed in close contact with a piece of n-type material, then a diffusion of electrons occurs from the region of high electron concentration (the n-type side of the junction) into the region of low electron concentration (p-type side of the junction). When the electrons diffuse across the p-n junction, they recombine with holes on the p-type side. However, in the absence of an external circuit the diffusion of carriers does not go on indefinitely because charges build up on either side of the junction create an electric field. The electric field promotes charge flow, known as drift current that opposes and eventually balances out the diffusion of electrons and holes. This region where electrons and holes have diffused across the junction is known as the depletion region because it contains practically no mobile charge carriers which are also known as the space charge region, although space charge extends a bit further in both directions than the depletion region.

Electric Field Equation

Electric field gives explanation on how Poisson equation came about from the differential form of gauss law. Increasing the doping concentration of donors or acceptors leads to more frequent collisions with the ionized dopant atoms which results to low mobility.

$\frac{dE}{dX} = \frac{\rho}{\varepsilon}$, Ɛ is the material permittivity

The charge density is ρ = q (p – n + $N_D^+ - N_A^-$) where N_D^+ is the ionized-donor density concentration, N_A^- is the ionized-acceptor density concentration and assuming that all dopants are ionized at room temperature, the equation will be ρ = q (p – n + N_D - N_A)

$\frac{d\varepsilon}{dX} = \frac{q}{\varepsilon}$ (p – n + $N_D - N_A$) is the equation of the electric field

Poisson equation gives the starting point in obtaining the qualitative solution for electrostatic variables in a semiconductor. Poisson's equation in equation 3 is a second order partial differential equation which depends on time for both electrons and holes and it contains electrostatic potential (∅) for a given charge (q) distribution.

$$\frac{d^2\emptyset_{(x)}}{dx^2} = \frac{q}{\varepsilon}[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)] \quad (3)$$

where ∅ is the electrostatic potential, q is the charge, ε is the dielectric constant of the medium, p is the free hole density, n is the free electron density, is N_D^+ the ionized-donor density, N_A^- is the ionized-acceptor density, n_t and n_p are trapped electrons density and trapped hole density. Poisson's equation is linked with how semiconductors behave in SCAPS because in semiconductors carriers are treated as a gas despite, they can diffuse and are transported as a gas. Electrostatic potential (∅) is the work needed in moving a unit charge from reference point to a specific point inside the field without producing acceleration. The charge (q) is used for each of the electrons here $[p(x) - n(x) + N_D^+(x) - N_A^-(x) + p_t(x) - n_t(x)]$. Effective density of states for conduction band (N_C) and valence band (Nv) does not change, because the only way it can change is by doping. When doping exceeds the effective density of states for conduction band and valence band we start to get degeneracy. Degeneracy is as a result of when the electrons are doped so high that the wave function overlaps. $N_D^+(x)$ And $N_A^-(x)$ are ionized, so as a result of their ionized state, n + N_A^- = p + N_D^+ which means that their positive and negative charges must be equal to each other.

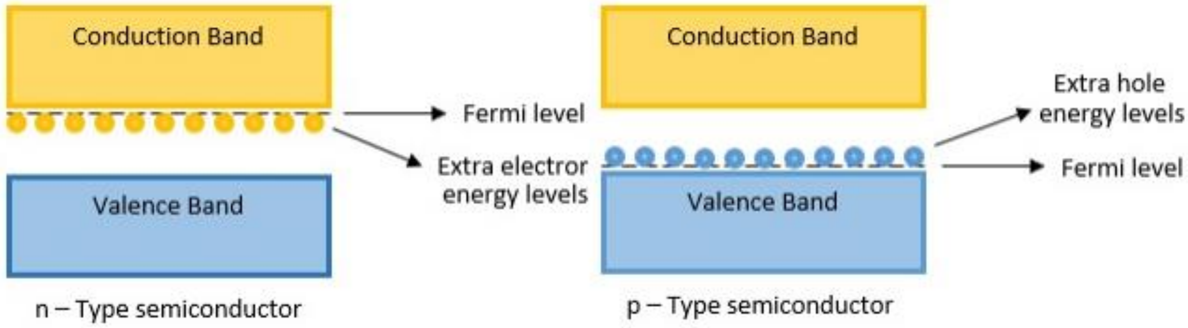

Figure 3: Illustration of n - type and p - type semiconductor on fermi level (Bube, 1998)

When doping an n type semiconductor with donors, the Fermi energy (E_F) is pulled up to the conduction energy (E_C), so as a result of that there will be more electrons and fewer holes but reverse is in the case of doping a p type semiconductor with acceptors as shown in figure 3. When doping increases, it result to ionized donor density (N_D^+), electrons that is close to N_D^+ want to diffuse backward that is from higher concentration to a lower concentration which creates an electric field between the electron (e-) moving forward and backward from the positive and negative direction. The electron that moves backward is called current diffusion while the electron that moves forward is called current drift i.e. $J_{DRIFT} = J_{DIFF}$.

Continuity equation for electrons and holes is linked with how semiconductors behave in SCAPS because every action undergone by charge carriers in a semiconductor device gives rise to a change in the carrier concentration with time. It governs how carriers behave with time when they are injected in semiconductors which contains some processes such as generation, recombination, current drift and mobility.

In addition, semiconductors contain majority and minority carriers indicate that the more abundant charge carriers are the majority carriers; the less abundant charge carriers are the minority carriers. Equilibrium carrier concentration can be increased through doping and the total number of carriers in the conduction and valence band is known as equilibrium carrier concentration.

For majority carriers, the equilibrium carrier concentration is equal to the intrinsic carrier concentration plus the number of free carriers added by doping the semiconductor. Under most conditions, the doping of the semiconductor is several orders of magnitude greater than the intrinsic carrier concentration, such that the number of majority carriers is approximately equal to the doping. At equilibrium, the product of the majority and minority carrier concentration is a constant, and this is mathematically expressed by Mass Law of Action.

$n_o p_o = n_i^2$

Where n_i is the intrinsic carrier concentration and n_o and p_o are the electron and hole equilibrium carrier concentrations.

Using the Law of Mass Action above, the majority and minority carrier concentrations are given as:

n-type: $n_o = N_D$, $p_o = \frac{n_i^2}{N_D}$

p-type: $p_o = N_A$, $n_o = \frac{n_i^2}{N_A}$

The above equations show that the number of minority carriers decreases as the doping level increases. For instance, in *n*-type material, some of the extra electrons added by doping the material will occupy the empty spots (i.e., holes) in the valence band, thus lowering the number of holes.

Continuity Equation for Electrons and Holes

In continuity equations, all terms used in the equation might look different but with single concept. The concept is conservation of some quantities, in which electromagnetism explain the conservation of energy but in semiconductors it explains about charge, that charge is neither created nor destroy but it can be transfer from one place to another. Continuity equation for electrons and holes is linked with how semiconductors behave in SCAPS because every action undergone by charge carriers in a semiconductor device gives rise to a change in the carrier concentration with time. It governs how carriers behave with time when they are injected in semiconductors which contains some processes such as generation, recombination, current drift and mobility. Continuity equation is all about the net change of carrier concentration is the difference between generation and recombination, plus the net current flowing in and out of the specified region as shown in equation 12 and 13.

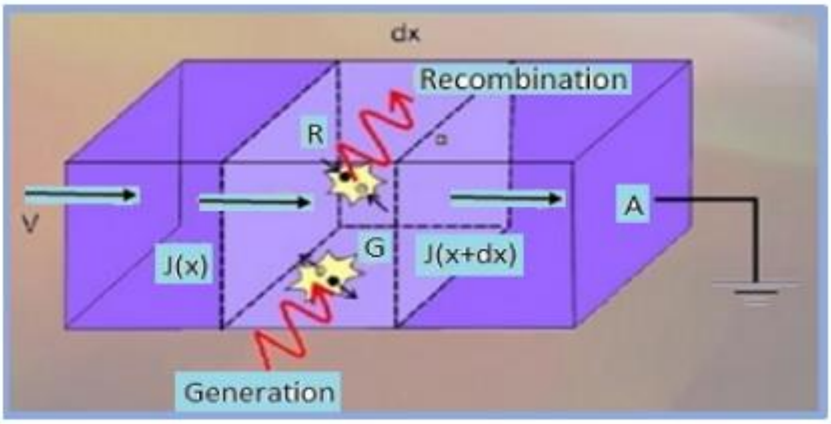

Figure 4: Conception view of the flow of electrons and holes in the equation of continuity (Bube, 1998)

$$\frac{\partial n}{\partial t} A \qquad (4)$$

The number of electrons within this box of volume AΔx is increasing and it can be represented in mathematical form as

$$\frac{\partial n}{\partial t} A\Delta x \qquad (5)$$

Where n = number of electrons, t = change with respect to time, A = cross sectional area, Δx = the thickness of the box and A x Δx = volume of box

Since the total number of electrons is increasing with respect to time in this box, at x the current density flowing in will be Jn(x) and at x the current density flowing out will be Jn(x + Δx).

Now the number of electrons flowing into this box can increase if only Jn(x) is higher than Jn(x + Δx) and the number of electrons flowing per unit time per unit area [Jn(x) A] can be written as

$$\frac{\partial n}{\partial t} A\ \Delta x = \frac{Jn(x)}{-q} A - \frac{Jn(x+\Delta x)}{-q} A \qquad (6)$$

The reason why the number of electrons in the box can increase is because of recombination and generation process which means that the carriers in this box will increase if the generation of electrons is greater than recombination as a result of the carriers flowing in is more than the carrier going out. So, equation 6 can also be written as

$$\frac{\partial n}{\partial t} A\ \Delta x = \frac{Jn(x)}{-q} A - \frac{Jn(x+\Delta x)}{-q} A + G_n A\ \Delta x - R_n A\ \Delta x \qquad (7)$$

G_n is the number of electrons generated into the box and R_n is the number of electrons recombined in the box.

To rearrange equation 7 by dividing through with AΔx, the following becomes

$$\frac{\partial n}{\partial t} = \frac{Jn(x+\Delta x)}{q\ \Delta x} - \frac{Jn(x)}{q\ \Delta x} + G_n - R_n \qquad (8)$$

$$\frac{\partial n}{\partial t} = \frac{1}{q}\left[\frac{Jn(x+\Delta x) - Jn(x)}{\Delta x}\right] \qquad (9)$$

Current density in equation 9 is represented in terms of space, now time will be included into equation 9

$$\frac{\partial n}{\partial t} = \frac{1}{q}\left[\frac{Jn(x+\Delta x, t) - Jn(x,t)}{\Delta x}\right] + G_n - R_n \qquad (10)$$

Let assume that there is a small box in which x tends to zero in equation 10 and $[\frac{Jn(x+\Delta x, t) - Jn(x,t)}{\Delta x}]$ is a standard partial differential equation that can be written as

$$\lim_{\Delta x \to 0} \frac{\partial n}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n - R_n \qquad (11)$$

Since equation 11 depends on space, it also depends on time. The following is continuity equation for electrons and is written in equation 12.

$$\frac{\partial n(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J_n}{\partial x} + G_n(x,t) - R_n(x,t) \qquad (12)$$

If the carriers in the box increase, its increases only because there is a difference in inflow and out flow and also, there is a difference in generation compare to recombination

$\frac{\partial n}{\partial t}$ can be negative because went is negative it means that the number of electrons concentration into this box is decreasing. In equation 6 the charge will be positive so that, the continuity equation for holes can be written in equation 13 as

$$\frac{\partial P(x,t)}{\partial t} = -\frac{1}{q}\frac{\partial J_P}{\partial x} + G_P(x,t) - R_P(x,t) \qquad (13)$$

RESULTS AND DISCUSSION

The reported work on temperature was in accordance with (Fahrenbruch *et al.*, 1989) which has conversion efficiency of 15.3%. In this simulation studies, 300K was chosen as the simulator operating temperature which is regarded as the room temperature. The performance of the solar cell is affected by the operating temperature during the course of this work; the operating temperature was varied between 270K and 600K to determine how the performance of perovskite solar cell, respond with this change on the operating temperature as compared with the experimental result obtained in (Du 2016, Usha *et al.*, 2017 and Mohammed *et al.*, 2020). The optimized PV parameters of the device were used with variation of operating temperature dependence of the solar cells as shown in Figure 5. The J_{SC} achieved is 30.73mA/cm^2 accompanying the highest PCE. The short circuit current increases slightly but decreases with temperature at 550K due to increase in photons possess sufficient energy to generate electron-hole pairs

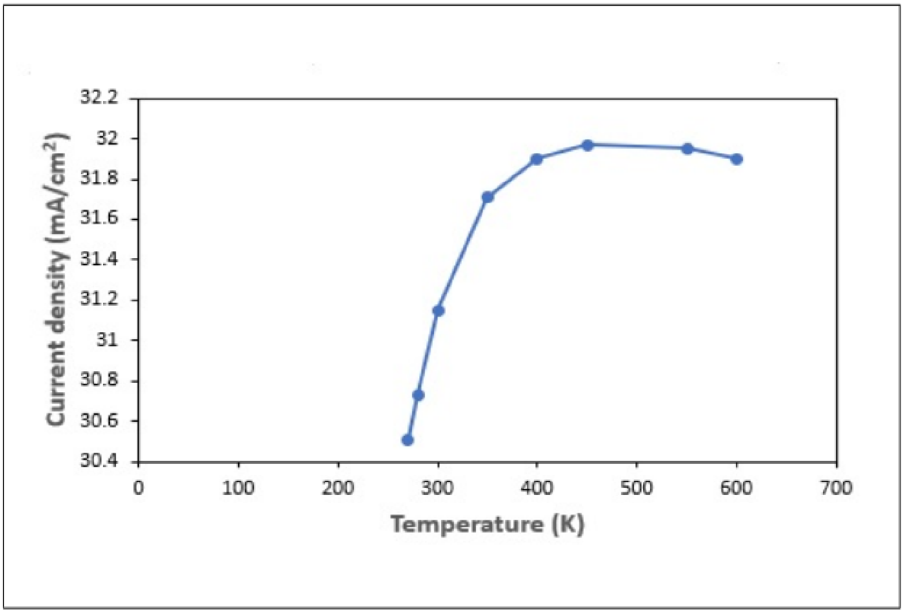

Figure 5: Current density as a function of temperature

When the voltage is low, the temperature variation has less effect on the current density which remains almost consistent. In a solar device, the parameter was influenced by starting with high increment of temperature having open circuit voltage of 0.96V at 270K but at 0.95V with 280K it was noticed that increasing the temperature leads to an unavoidable decrease of the voltage. The optimized PV parameters of the device were used with variation of operating temperature dependence of the solar cells as shown in Figure 6. The V_{OC} is 0.95V accompanying the highest PCE.

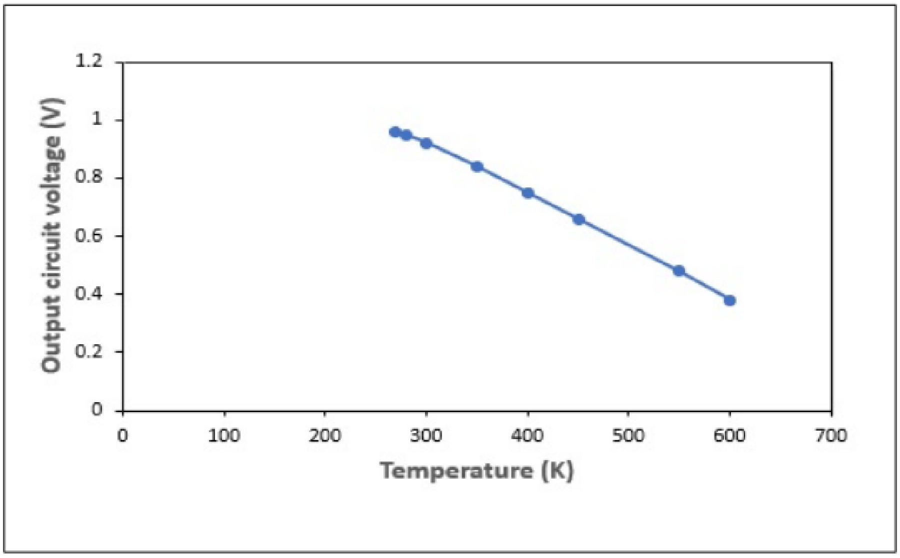

Figure 6: Output circuit voltage as a function of temperature

The optimized PV parameters of the device were used with variation of operating temperature dependence of the solar cells as shown in Figure 7. The Fill factor increases from 81.68% at 270K but began to decrease at 82.79% with increasing temperature from 350K to 600K because of the level of charge carriers. The FF is 82.80% accompanying the highest PCE.

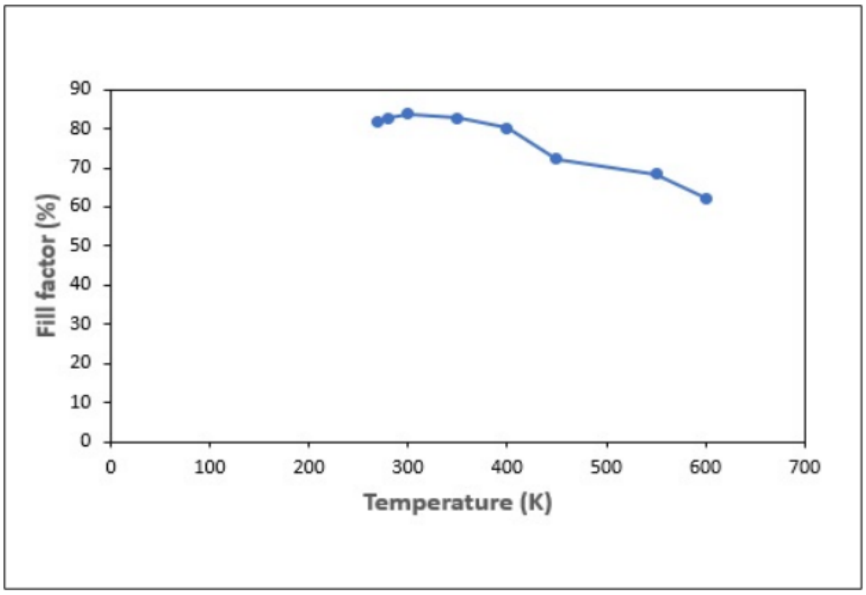

Figure 7: Fill factor as a function of temperature

From the simulation results, it can be said that efficiency decreases with the increase of temperature because the electron and hole mobility changes with temperature. The optimized PV parameters of the device were used with variation of operating temperature dependence of the solar cells as shown in Figure 8. The highest PCE achieved is 24.25% accompanying by the remaining solar cell parameters FF of 82.80%, J_{SC} of 30.73mA/cm^2, V_{OC} of 0.95V.

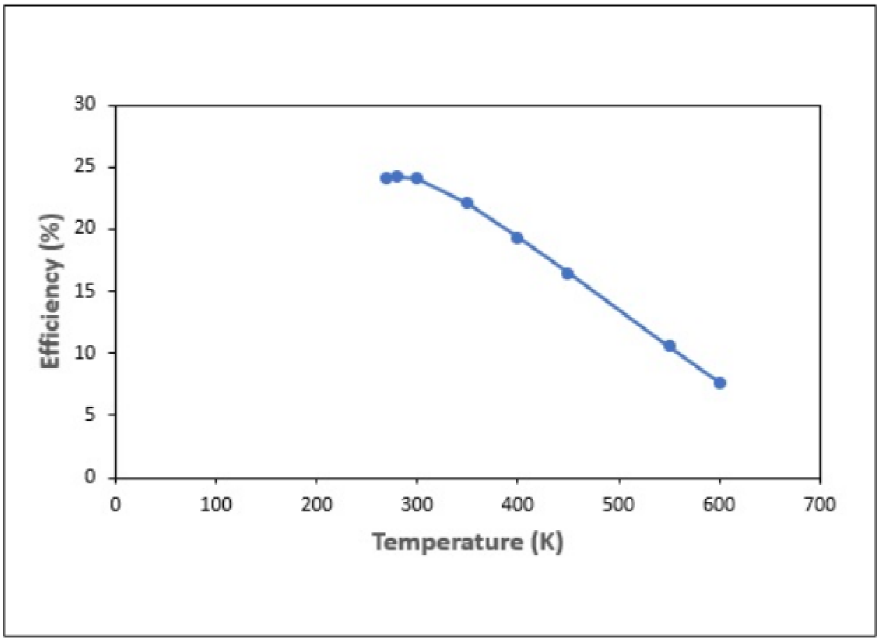

Figure 8: Power conversion efficiency as a function of temperature

The J-V curves were obtained at light for the temperatures 270K to 600K which shows enhancement in the short-circuit current from the photo. Figure 9, J-V curve as a function of temperature, confirms the variation of J_{SC}, V_{OC}, FF, efficiency and hence resistance in the solar cell devices. The performance of the solar cells is influenced by operating temperature. At temperature above room temperature, the solar cells have exhibited higher performance and below room temperature all PV parameters have moderate values because the efficiency was decreasing as shown in table 1. The temperatures above room temperature are not beneficial to the overall performance because at high temperature the carrier concentrations, mobility of the charge carries and resistance of the materials would be greatly affected which would ultimately alter PV parameters.

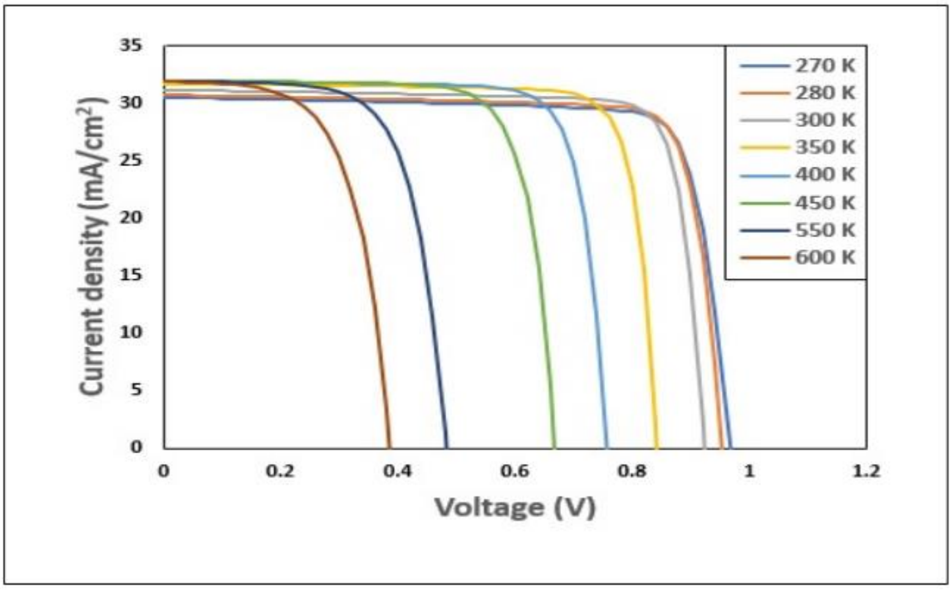

Figure 9: J-V curve as a function of temperature

Table 1: Dependence of solar cell performance on temperature

Tempertaure (K)	J_{SC}(mA/cm^2)	V_{oc}(V)	FF(%)	PCE(%)
270	30.51	0.96	81.68	24.12
280	30.73	0.95	82.80	24.25
300	31.15	0.92	83.72	24.06
350	31.71	0.84	82.79	22.11
400	31.90	0.75	80.17	19.35
450	31.97	0.66	72.20	16.48
550	31.95	0.48	68.45	10.54
600	31.90	0.38	62.26	7.67

CONCLUSION

Tin perovskite-based solar cells have been successfully simulated using SCAPS-1D. It was observed that with increment in the temperature from 270K to 600K. The thickness of absorber layer was changed from 0.03µm to 1.5µm; the better performance of the device was achieved at the thickness of 0.9 µm as in which were used in comparing with effect of temperature on this study. The result shown in indicates that all the materials used was not expensive especially the back-metal contact (Ag), HTM (Cu_2O) and ETM (CdS) as compared with which some of the materials are expensive (Au, TiO_2 etc.). The highest PCE achieved is 24.25%, FF of 82.80%, J_{SC} of 30.73mA/cm^2, V_{OC} of 0.95V. These simulation results illustrate that in a doped material, the minority charge carriers have a short diffusion length but the majority charge carriers have a long diffusion length which will largely affect the device performance.

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