SCAPS Simulation for Perovskite Solar Cell

R. Tala-Ighil Zaïr[1,2,*], C. Oudjehani[1] and K. Tighilt[1]

[1]*Institute of Electrical & Electronic Engineering, University M'hamed Bougara Boumerdes, Route de l'indépendance, 35000, Algeria*

[2]*Research Unit on Materials, Processes & Environment, University M'hamed Bougara Boumerdes, Route de l'indépendance, 35000, Algeria*

Abstract: Perovskite solar cells are keeping a very high interest in the solar energy world, with an efficiency in constant rise each year. In this study, we designed a tin-based (Hole Transport Material) HTM perovskite solar cell with the novel architecture **Au/$CH_3NH_3SnI_3$/TiO_2/ZnO: Al**. A simulation has been carried-out by using the SCAPS-1D solar cell capacitance simulator, which is well adapted to study the solar cell behavior. Through the software tool, we have studied the absorber's layer thickness effect and the model operating temperature by plugging many varied parameters. The encouraging results of: 20.08% conversion efficiency, 32.76mA/cm² short-circuit current density (Jsc), 0.827 V open circuit voltage (Voc), and a fill factor (FF) of 74.06%, are predicted with the obtained optimal parameters.

The results indicate the high aptitude of lead free & HTM perovskite to achieve high efficiency and become a good alternative for the traditional solar cells in the future.

Keywords: Solar Cells, Perovskite, SCAPS, $CH_3NH_3SnI_3$.

1. INTRODUCTION

The perovskite based solar cells represent a real alternative compared to the other types. This is especially due to the low cost material, the lowest thickness of the absorber layer which permits to manufacture a high number of solar cells with few amount of matter [1]. With more and more satisfactory results every year, perovskite are believed to be the best possible successor to silicon solar cells in the future [2]. The main purpose of this work, is the study of lead-free, therefore toxicity free, and HTM free perovskite solar cell in order to obtain the best perovskite structures which are eco-friendly. The simulation tool SCAPS-1D software has been used [3, 4], and **$CH_3NH_3SnI_3$** perovskite solar cell has been simulated [5].

Perovskite solar cells have shown their capacity to be the best potential candidate for the new solar cells generation, as the photoelectric power conversion efficiency of these cells has jumped from 3.8% in 2003 to 25.2 % in 2020 [6]. They have been rapidly developed due to the extensive attention they aroused in scientists worldwide, because of their high efficiency and low cost. In this paper, we will dig deeper into the structure and simulation process for the proposed perovskite solar.

*Address correspondence to this author at the Institute of Electrical & Electronic Engineering, University M'hamed Bougara Boumerdes, Route de l'indépendance, 35000, Algeria; Tel: +21324795758;
E-mail: r.tala-ighil@univ-boumerdes.dz

2. INPUT SIMULATION DATA

Perovskite Solar Cells: The Detailed Structure

Perovskite is a type of mineral that was found in the Ural Mountains and named after Lev Perovskite (the founder of Russian geographical society); true perovskite is composed of Calcium, Titanium and Oxygen in the form $CaTiO_3$.

A Perovskite structure is any compound that has the form ABX3, and the same Crystallography as the Perovskite mineral.

The crystal structure of the form ABX3 is represented below:

The perovskite crystal structure has the form ABX3. Both the two structrures are the same [7].

The first perovskite applied to solar cells was used in 2012.

The materials ABX3 is composed of:

A = an organic Cation - methylammonium ($CH_3NH_3^+$) or Formamidinium ($NH_2CHNH_2^+$).

B = A big inorganic Cation - usually lead (II) (Pb^{2+}).

X_3= A slightly smaller Halogen Anion – usually Chloride (Cl^-) or Iodide (I^-) [7].

The classical perovskite solar cells structure has the (n-i-p) type: The glass is used as the substrate, on

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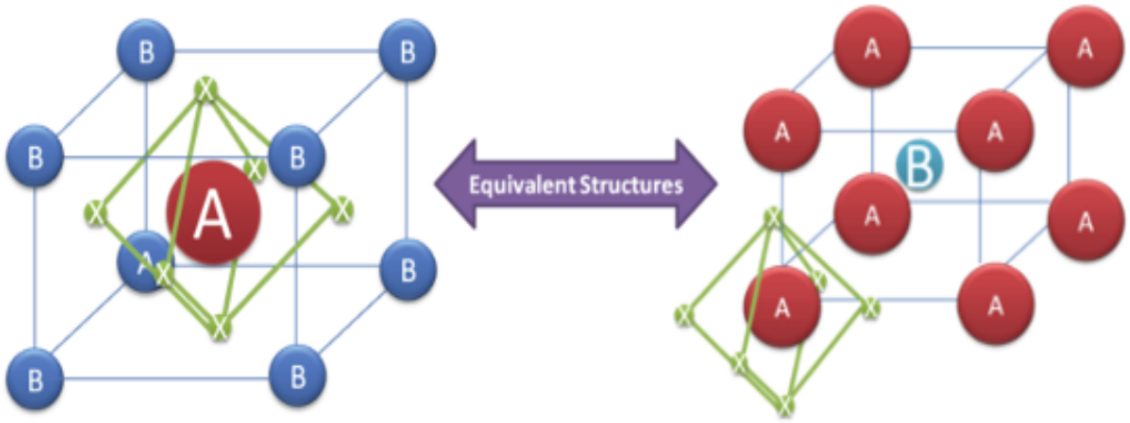

Figure 1: The crystal structure of the form ABX3 [7].

which is deposited the fluorine doped tin oxide FTO thin film, followed by titanium dioxide, considered as the n-type semiconductor that conducts electrons. They form the anode.

The perovskite material, for example **Metal Amonium Lead Triodide (MAPbI3)** plays the role of the absorber. The Spiro-OMeTAD is the p-type layer.

3. RESULTS & DISCUSSIONS

SCAPS-1D **"Solar Cell Capacitance Simulator one Dimension "** is a one dimensional solar cell simulation program developed at the Department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium [9].

3.1. Working with SCAPS

SCAPS is a software that contains many panels on which the user can insert the different solar cell characteristics. The results are calculated and sketched. There are three major panels: **action panel**, solar **cell definition panel** and the **energy band panel**.

We used $CH_3NH_3SnI_3$ as the absorber layer, TiO_2 as electron transport material (ETM), ZnO: Al as front contact and Au as back contact (see Figure **4**)

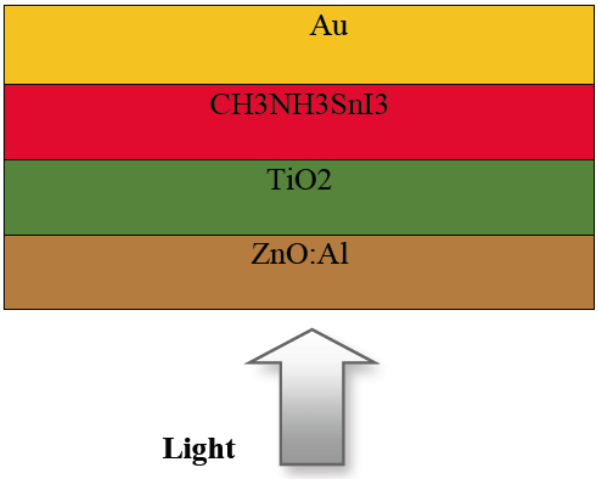

Figure 3: architecture of the studied perovskite solar cell.

3.2. Insertion of the Input Data for HTM and Lead free Perovskite Solar Cell

In the Table **1** below are listed all the materials' parameters needed to perform the simulation:

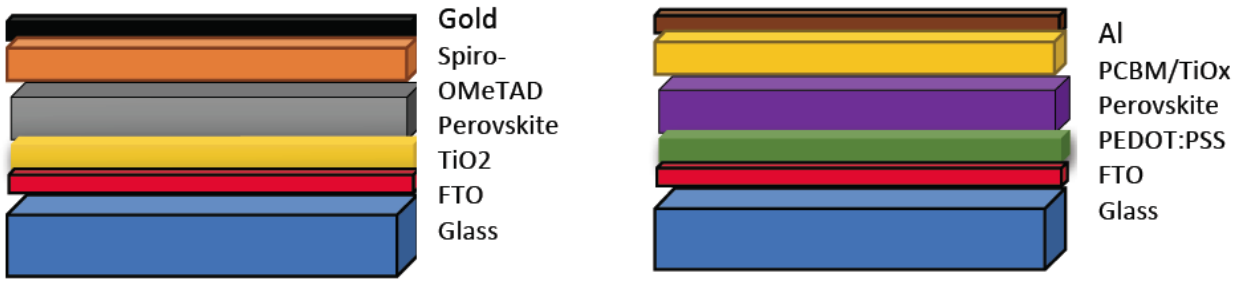

Figure 2: the normal and inverted structure of Perovskite solar cells [8].

Table 1: Materials Parameters of the Simulated Solar Cell

	$CH_3NH_3SnI_3$	TiO_2	ZnO:Al
Thickness (μm)	0.7	0.04	0.24
Band Gap (eV)	1.3	3.2	3.3
Electron affinity (eV)	4.17	3.9	4.6
Dielectric permittivity (relative)	6.5	9	9
Electrons in CB (cm^{-3})	1×10^{18}	1×10^{21}	2.20×10^{18}
VB (cm^{-3})	1×10^{19}	2.00×10^{20}	1.80×10^{19}
Electron thermal velocity (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}
Hole thermal velocity (cm/s)	1×10^{7}	1×10^{7}	100
Electron mobility (cm^2/Vs)	1.60	20.0	100
Hole mobility (cm^2/Vs)	1.60	10.0	20.0
ND (cm^{-3})	0	1×10^{19}	1×10^{18}
NA (cm^{-3})	3.20×10^{15}	1.0	0

-The resulting J-V curve obtained under T=300K and default light characteristics is shown below:

3.3.1. Effect of the Absorber Layer Thickness on the Cell Performance

In this part, the ($CH_3NH_3SnI_3$) absorber layer's thickness effect has been investigated. The main objective of this simulation is to find the optimal thickness that result in optimal characteristics.

The figure below shows the simulated parameters (solar cell characteristics) of the perovskite solar cell as the thickness of the perovskite material varies.

The absorber layer thickness is varied from 0.2μm to 0.7μm. It is found that the characteristics are sharply increasing as the thickness increases, due to the increase in the optical path length where more photons have chance to be absorbed and generate electron

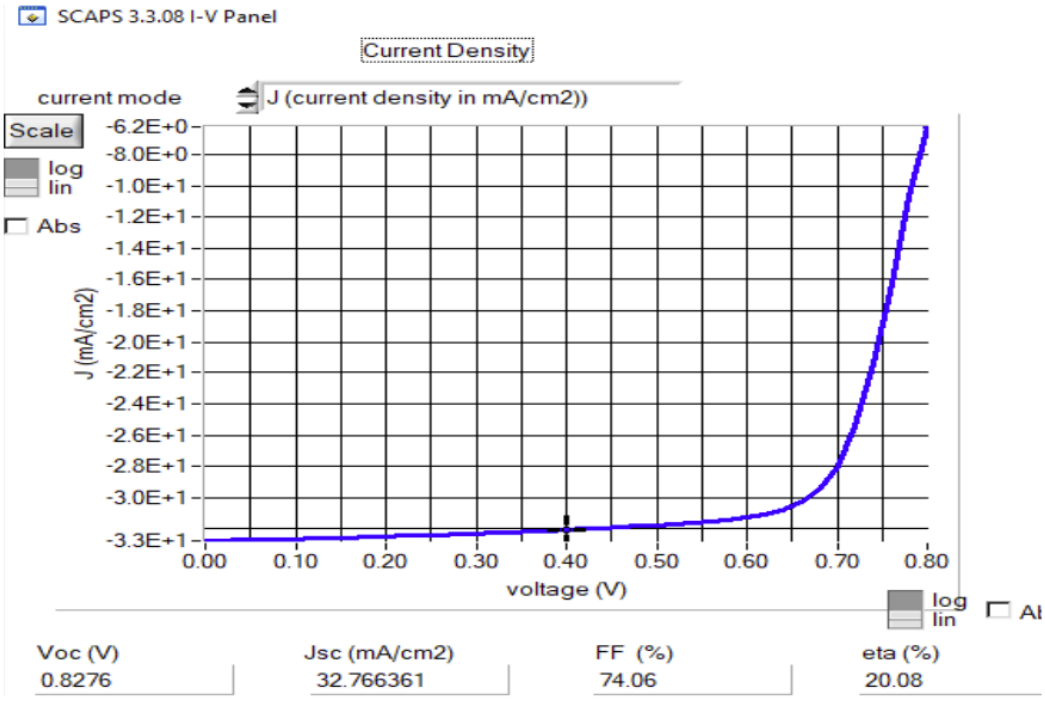

Figure 4: J-V curve of the studied solar cell at T=300K.

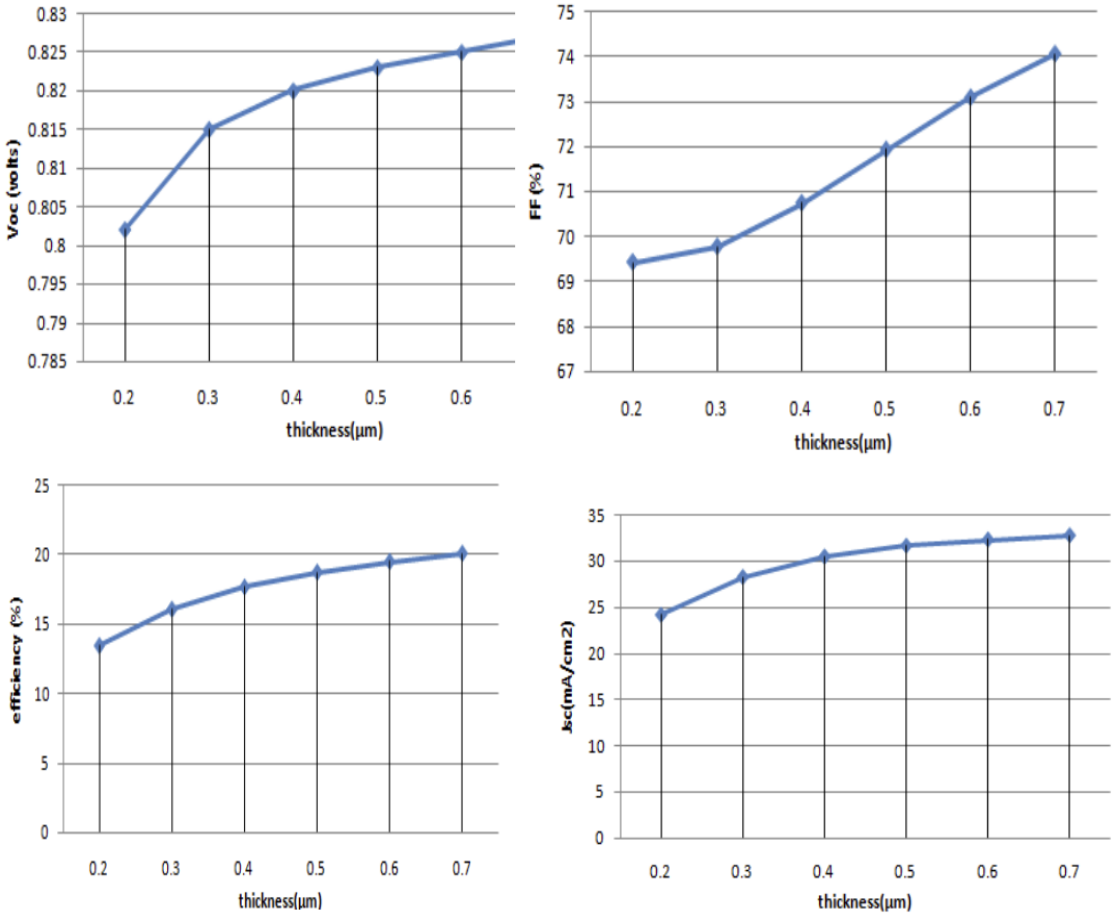

Figure 5: solar cell characteristics variations as a function of absorber layer thickness.

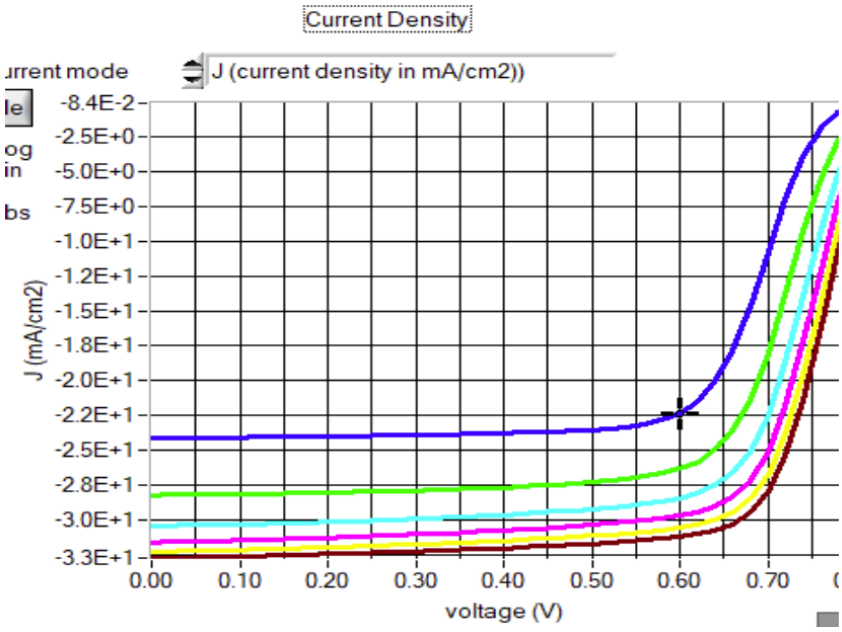

Figure 6: J-V curve for varying thickness.

hole pairs; the values PCE=20.08%, FF=74.06%, Jsc=32.76mA/cm², Voc=0.827 V were achieved at thickness = 0.7µm.

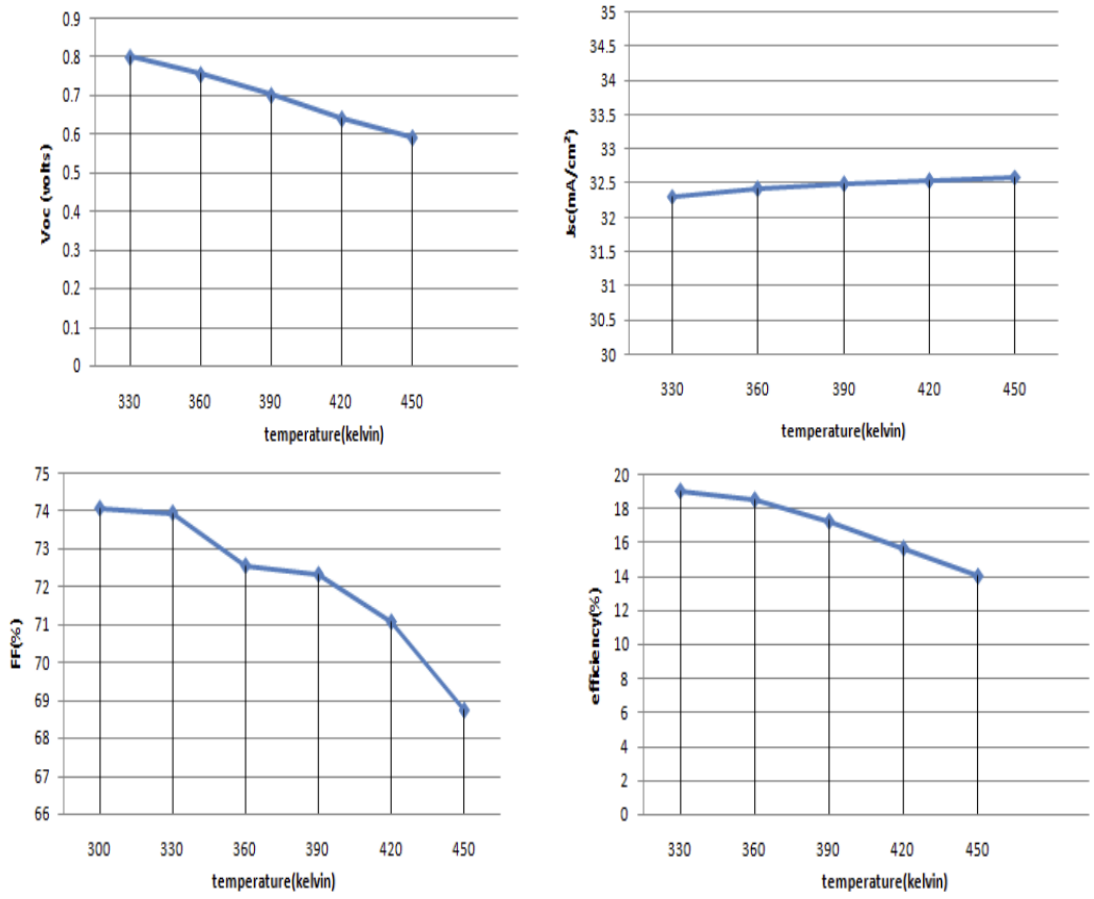

Figure 7: solar cell characteristics variations as a function of working temperature.

3.3.2. The Effect of the Working Temperature on the Performance

Like all other semiconductor devices, solar cells are sensitive to temperature, which exceeds 300K when installed outdoors. This is why, for that, it would be important to examine the temperature effect on the solar cell performance.

(Figure **7**) shows the variation of Jsc, Voc, FF and the efficiency as a function of temperature.

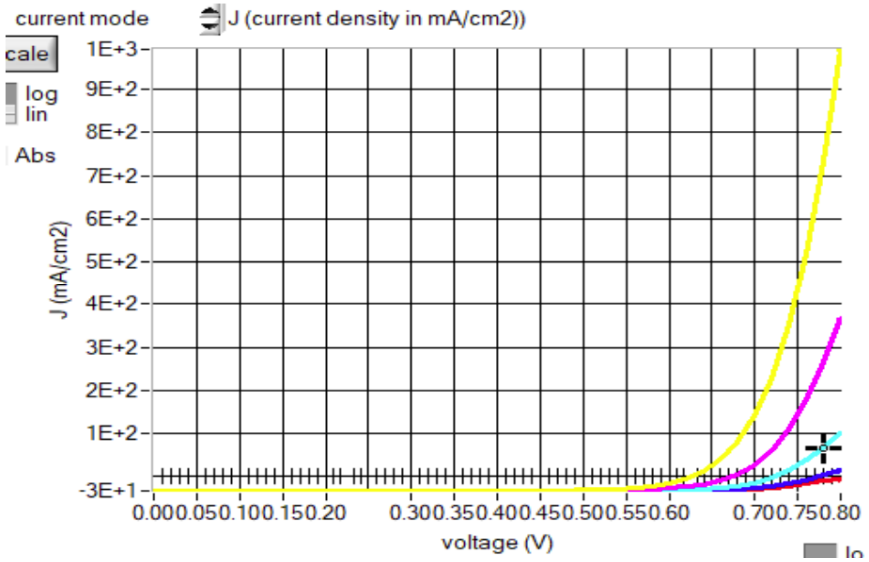

Figure 8: J-V curve for varying temperature.

From the graphs, one can remarks that as the temperature increases the short current density rises slightly. It is essentially due to the slight band gap reduction. Where as the open circuit voltage decreases rapidly due to its dependency on the saturation current (which depends on temperature), making it the most affected characteristic ; we also note that the fill factor and the efficiency decrease as well, hitting minimum values of Voc = 0.591 V, FF=68.74% and PCE=14.06% at T=450K.

4. CONCLUSION

HTM and Lead free Perovskite solar cell has been simulated using SCAPS-1D. The thickness of the absorber layer and the working temperature have been varied. Very interesting results were obtained with an efficiency of 20.08 %. We concluded that in order to have high efficiency the absorber layer's thickness should be thick enough to absorb a large amount of photons and the temperature should be as cool as possible.

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