

Numerical Study of Based Perovskite Solar Cells by SCAPS-1D

Abdelhadi SLAMI, Mama BOUCHAOUR and Laarej MERAD

Abstract—This work deals with the design and analysis of lead-based Perovskite solar cells. The architecture consists of Glass/TCO/Buffer layer (TiO_2)/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ /Spiro-MeTAD/metal back contact (Aluminium).

To study the efficiency and the performances of this solar cell, SCAPS-1D software is used in the simulation. The influence of defect density, absorber layer thickness, and working temperature on the performance of the device is presented.

The optimized PCS is obtained for the absorber layer thickness of 900 nm, the defect density of 10^{13} cm^{-3} and the 300K operating temperature. The efficiency greater than 30% is obtained.

Keywords: SCAPS-1D, Perovskites solar cell, Simulation, Efficiency.

I. INTRODUCTION

In recent years, Perovskite Solar Cells (PSCs) have shown a great performance because of their low cost fabrication than traditional solar cells. It officially, entered the world of photovoltaics with a yield of 12% (2012) [1]. Since then, the yield of PSC has increased very rapidly reaching the value of 22% (2016) [2-4]. Owing the multilayer architecture of PSCs, interface not only has a main role to play in performance but influences long term stability.

By varying $\text{CH}_3\text{NH}_3\text{PbI}_3$, high efficiency is predicted. Thus, several simulations are made in order to study the effect of various parameters on the efficiency of solar on $\text{CH}_3\text{NH}_3\text{PbI}_3$ cells.

In this architecture, the effect of absorber layer properties (thickness, defect densities) and the influence of temperature on the performance of the device is studied and analyzed.

II. NUMERICAL MODELLING AND DEVICE SIMULATION

The adopted planar hetero-junction architecture is a typical $\text{CH}_3\text{NH}_3\text{PbI}_3$, based solar cell structure. The cell consists of an absorber layer and at the top p-type (Spiro-OMeTAD) (HTM) and n-type (TiO_2 -ETM) arranged at the bottom side as shown in figure 1.

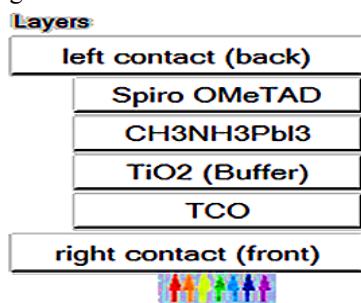


Fig. 1 Schematic representation device architecture (Glass/TCO/ TiO_2 -ETM/ $\text{CH}_3\text{NH}_3\text{PbI}_3$ /Spiro OMeTAD/Al)

Figure 2 explains the simulation process using SCAPS.

SCAPS is a one dimensional solar cell simulation program developed at the department of Electronics and Information Systems (ELIS) of the University of Gent, Belgium. It allows to simulate the behavior of photovoltaic structures. Since that, there are several modifications in this software such as the capability to work with crystalline solar cells (c-Si and GaAs, family) and amorphous cells (a-Si and micro-morphous Si) [5]. This simulator has the largest number of AC and DC electrical measurements which can be calculated in dark and light illumination and also at different temperatures. It (SCAPS) solves the Basic semiconductor equations in 1-Dimension under steady state condition.

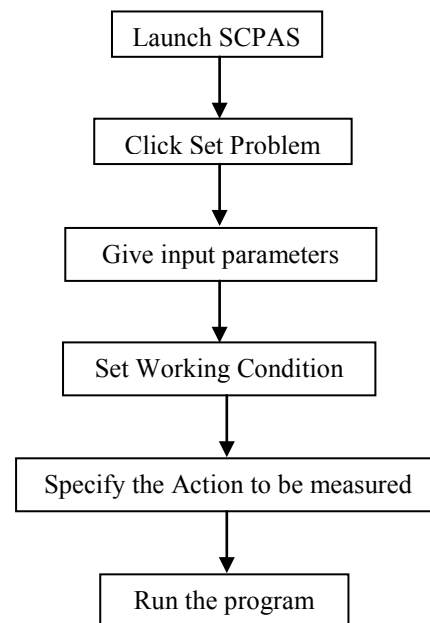


Fig. 2. SCAPS working procedure.

All simulation parameters are carefully selected from those reported in experimental data and other theoretical results [6-9]. The individual materials parameters for Spiro-OMeTAD, $\text{CH}_3\text{NH}_3\text{PbI}_3$, TiO_2 and TCO (SnO_2 :F) have to be entered in terms of bandgap (E_g), electron affinity (χ), dielectric permittivity (ϵ), conduction band density of states (NC), valence band density of states (NV), electron mobility (μ_n), hole mobility (μ_p), donor density (NA), acceptor density (ND). Table 1 summarizes all the parameters used in the simulation.

Parameters	TCO SnO ₂ :F	TiO ₂ (Buffer) (ETM)	CH ₃ NH ₃ PbI ₃	Spiro-OMeTAD (HTM)
Thickness/nm	500	50	900	350
Band gap energy E _g /ev	3.5	3.2 [13]	1.55 [14]	3.17[17]
Electron affinity χ /ev	4	4 variable	3.90 [15]	2.05 variable
Relative permittivity ϵ_r	9	9	6.5 [16]	3
Effective conduction band density N _c /cm ⁻³	2.20 x 10 ¹⁸	1.00 x 10 ¹⁹	1.80 x 10 ¹⁸	10 ²⁰
Effective valence band density N _v /cm ⁻³	1.80 x 10 ¹⁹	1.00 x 10 ¹⁹	1.80 x 10 ¹⁹	10 ²⁰
Electron mobility μ_n /cm ² /V.s	20	0.02	0.5	2
Hole mobility μ_p /cm ² /V.s	10	2	0.5	0.01
Donor concentration N _D /cm ⁻³	2.00 x 10 ¹⁹	1.00 x 10 ¹⁹ [13]		
Acceptor concentration N _A /cm ⁻³			1.00 x 10 ¹⁹	1.00 x 10 ¹⁹
Defect density N _i /cm ⁻³	1.00 x 10 ¹³	1.00 x 10 ¹⁶	1.00 x 10 ¹³	1.00 x 10 ¹³

Table 1. Simulation parameters of CH₃NH₃PbI₃ PSC [10, 11]

A. Current – Voltage Curve

The final model contains thickness of absorber layer as 0.9 μ m and the defect density as 10¹³ cm⁻³. The doping levels of HTM and ETM are set as 10¹⁹ cm⁻³. Fig 3. represents the characteristic of Perovskite solar cells of the final J-V. The open circuit voltage (V_{oc}) is 0.67V, Short circuit current density (J_{sc}) is 59.78mA/cm², Fill factor is 74.94%, and PCE is 30.35%.

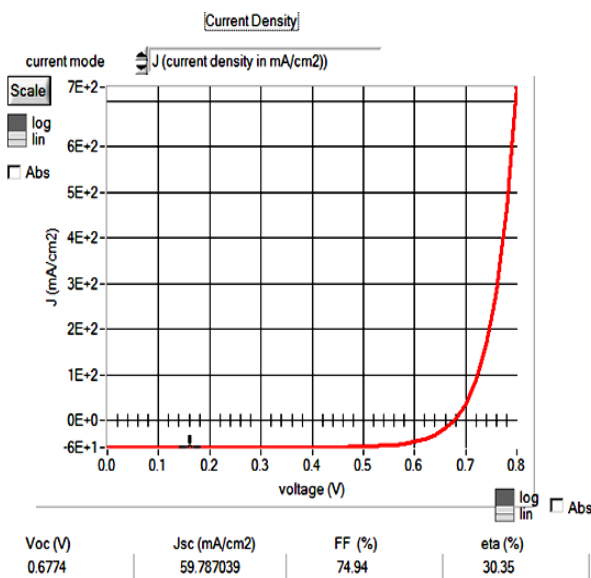
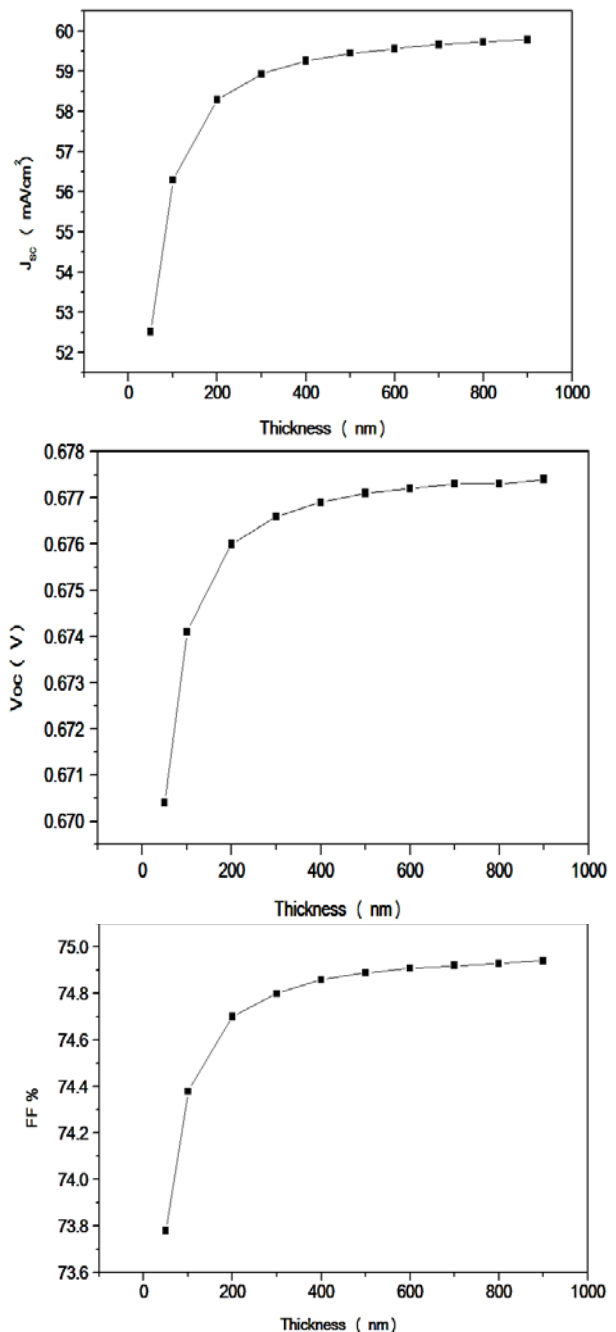


Fig. 3 Simulated J-V graph using SCAPS-1D

B. Influence of absorber layer thickness on the I-V

Absorber layer thickness plays a major role in determining the efficiency of the device [9]. The simulated parameters such as PCE, FF, J_{sc}, V_{oc} of the CH₃NH₃PbI₃ solar cells, with varying Perovskite thickness is as shown in Fig 4. Maximum PCE is obtained for 30.35%. This result is achieved with J_{sc}=59.78mA/cm², FF=74.94%, V_{oc}=0.6774V when the thickness reaches 900 nm.



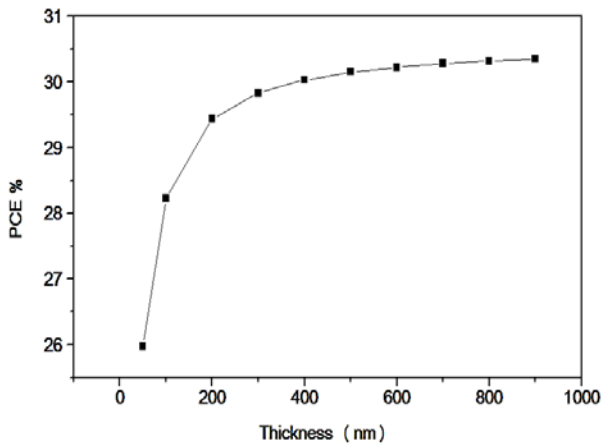


Fig. 4 Variation of solar cell parameters with thickness of absorber layer

To optimize the thickness for a good efficiency, the thickness of Perovskite layer from 50nm-900nm is varied. From the above graph (Fig.4: thickness versus efficiency), the efficiency rapidly increases from 50 nm till to 200nm up of 200nm, it slowly increases.

The increase of efficiency with increasing thickness represents the increase in the generation of the electron-hole pairs in the absorber layer. The efficiency slowly increases representing the decreases of recombination and a lot extraction rate of electron and hole pairs. The main reason for the increase of efficiency with the increase of thickness is the increase of optical density [3].

C. Influence of defect of the active layer on the I-V

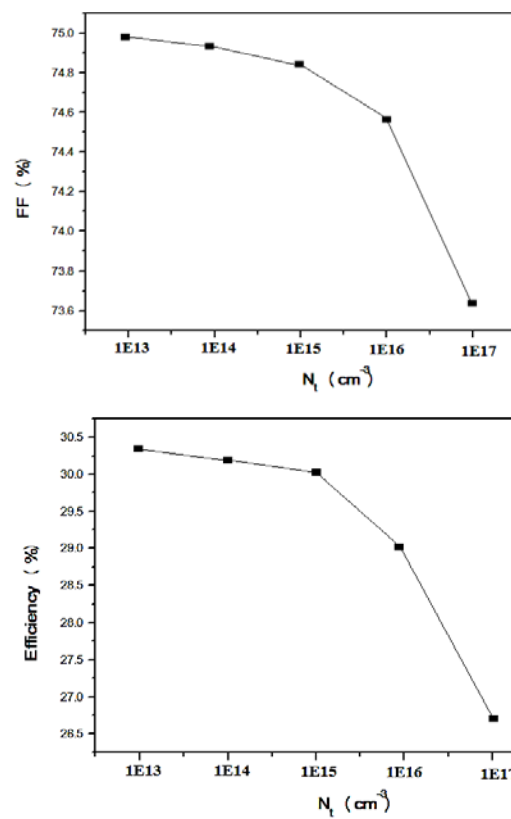
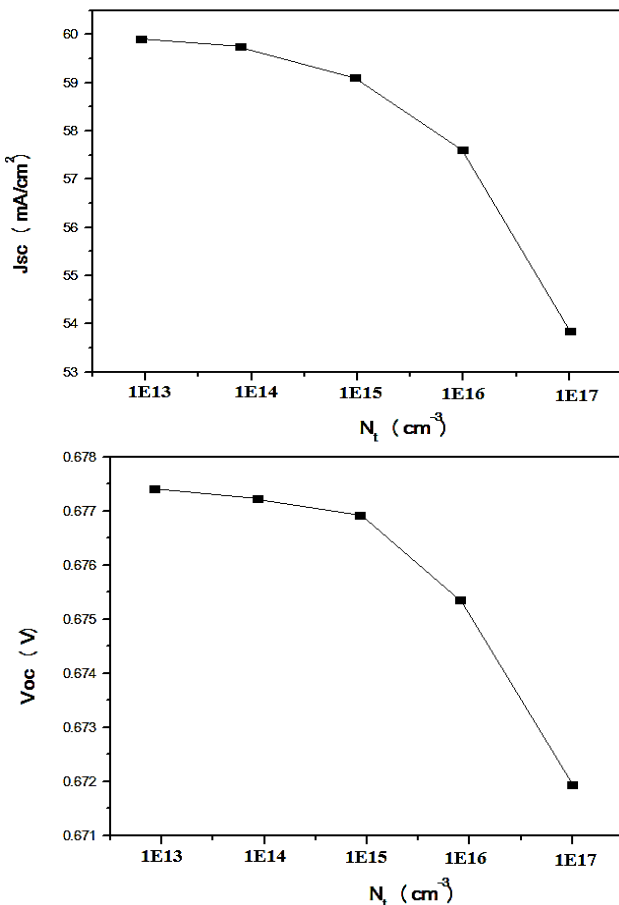
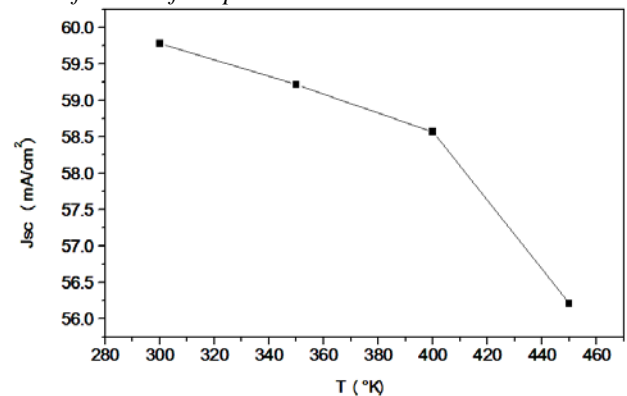


Fig.5 represents the variation of PV parameters with the defect densities (cm^{-3}). Generation, recombination, transportation process occurs inside the absorber layer, so the absorber layer quality and defect parameters greatly effect the device performance [18]. There are several defects such as vacancies, dislocation and grain boundaries which are always present in the absorber and HTM layer. These defects influence carrier recombination, reduction in lifetime and carrier mobility [11]. In the simulation model, the defect density is varied from 10^{13} cm^{-3} to 10^{17} cm^{-3} . It was observed that, if the defect density absorber layer is increasing from 10^{13} cm^{-3} , to 10^{17} cm^{-3} , the photovoltaic parameters randomly decreases and at 10^{17} cm^{-3} the PCE reaches to the 26.65 % and fill factor is 73.65 %, $V_{oc}=0.6715 \text{ V}$, $J_{sc}=53.88 \text{ mA}/\text{cm}^2$. The minimum defect density of the absorber layer is predicted as 10^{13} cm^{-3} , at this condition the maximum attainable PV parameters are efficiency: 30.35%, Fill factor: 74.94%, $J_{sc}=59.78 \text{ mA}/\text{cm}^2$, $V_{oc}=0.6774 \text{ V}$.

D. Influence of temperature on the I-V



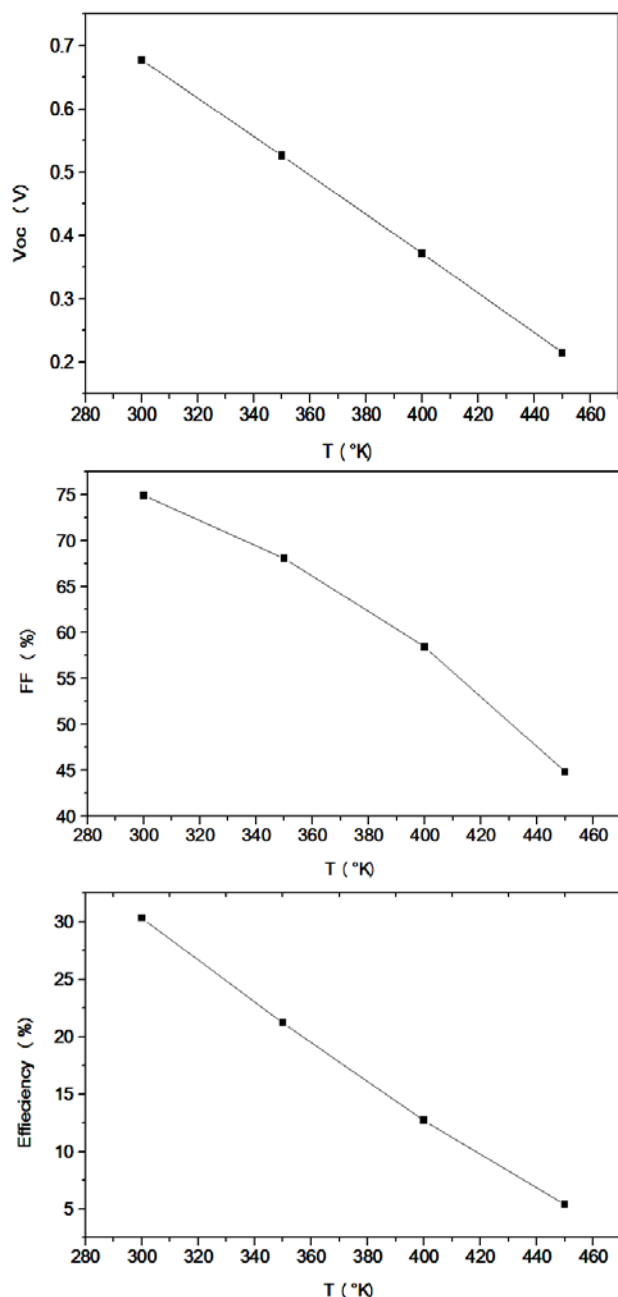


Fig.6 Variation of solar cell parameters with the operating temperature.

Temperature also influences the performance of a solar cell device. Generally, the testing temperature of a solar cell device is 300°K, but at the installed conditions, the working temperature is more than 300°K [17]. To understand the effect of temperature on the electrical performance of a solar cell, the temperature of the simulated model varied from 300K to 450K. The changes in the characteristics are given in Fig.6. It is observed that the temperature decreases; there is a drop to 5.42%. Increasing temperature may lead to the more stress and deformation resulting in increased interconnectivity between the layers. Decrease in diffusion length increases of series resistance, by this fill factor and efficiency will be decreased [18]. To achieve good efficiency the optimum temperature of the simulated model is set to be 300K. At this temperature the maximum achievable efficiency of the model is 30.35%, fill factor is 74.94%, $J_{sc} = 59.78 \text{ mA/cm}^2$ and $V_{oc} = 0.6774 \text{ V}$.

III.CONCLUSION

The lead $\text{CH}_3\text{NH}_3\text{PbI}_3$ Perovskite solar cells with different parameters are analyzed by using one-dimensional device simulation in this work (SCAPS-1D). TiO_2 material is proposed as the Electron Transport Layer (ETL) for lead $\text{CH}_3\text{NH}_3\text{PbI}_3$ based Perovskite solar cells. The thickness and doping level of the active layer are varied to study the optimized performance. Simulated results reveal that the efficiency of this solar cell is 30.15%. In future, the results of this proposed structure need to be validated through physical fabrication and further study.

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