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ORIGINAL ARTICLE

Thickness Variation Study of Perovskite Layer Over the Range 100-1300 nm and Its Influence on the Performance of Perovskite Solar Cells Using SCAPS Software

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ABSTRACT

The thickness of the light-absorbing layer plays a critical role in determining the metrics of perovskite solar cells (PSCs). Herein, the simulation of Tin-based perovskite solar cells using one-dimensional Solar Cell Capacitance Simulator (SCAPS-1D) software was reported systematically. The effect of absorber thickness on the performance metrics was investigated. The variation of the thickness of the absorber layer was varied from 100 nm to 1300 nm. The results of the initial device showed performance in Short Circuit Current Density (J_{sc}) of 20.991 mAcm^{-2}, Open Circuit Voltage (V_{oc}) of 0.741 V, Fill Factor (FF) of 54.048%, and Power Conversion Efficiency (PCE) of 8.256%. The Quantum Efficiency (QE) of the device shows strong activity within the visible region of the electromagnetic spectrum. Controlling the perovskite layer thickness, results to best PCE of 8.382%, J_{sc} of 21.166 mAcm^{-2}, V_{oc} of 0.741 V and FF of 53.439% at thickness of 0.5 µm. When the optimized result is compared with the initial device, an improvement of ~1.02 times in PCE, ~ 1.01 in J_{sc} was obtained over the initial device. The results obtained show that, for better PSCs performance, careful selection of the thickness of the absorber layer is important for good photon absorption.

1 Introduction

The perovskite material is an important part of the PSCs, playing a significant role in absorbing light, generating photo-stimulated carriers, and injecting these carriers into the network. Hybrid perovskites are defined on the basis of AMX_3 crystal structure, where A is an organic cation, for example, methylammonium or formamidinium, M is a metal and X is a halogen atom. As these perovskite materials are ambipolar, they can allow the conduction of both electrons and holes simultaneously.

Also, they show high electron and hole mobilities, which have attained several cm^2/Vs [1, 2]. The hole mobilities are considered much higher (164 ± 25 cm^{2}V^{-1}s^{-1}) than the mobilities demonstrated by electrons (24.8 ± 4.1 cm^{2}V^{-1}s^{-1}) for methylammonium lead triiodide ($CH_3NH_3PbI_3$) as determined using Space charge limited current method, in agreement with results from Hall effect and time of flight [3, 4].

Even though lead (Pb) perovskite absorbers have demonstrated good absorbing abilities and can efficiently be used in perfectly developed devices, the environmental effect it poses to the ecosystem has resulted to great threat in achieving a clean energy system.

The replacement of Tin (Sn) that is less toxic than lead is a good alternative for ecofriendly PSCs [5, 6]. When compared with the Pb-based counterpart absorber, the synthesis of Sn-

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based perovskites encourages perovskite material with lower band gap (E_g) [5, 7-9].

Simulation study in PSC is as crucial as the experimental study if optimized and enhanced devices must be reached. Amongst the several research works demonstrated recently, Muhammed et al. [10] simulated the influence of doping concentration of absorber layer, influence of electron affinity of ETM and HTM, effect of absorber thickness, influence of defect density, influence of hole mobility on the overall PSC performance and predicted a *PCE* value of 20.35%.

Islam et al. [5] published a theoretical study of the impact of amphoteric defect density in the absorber layer, effect of interface defect states, metal work function and effect of doping density of the TiO_2/$MASnBr_3$ heterojunction on the physical parameters of the Tin-based PSC and achieved a *PCE* of 21.66%.

TiO_2 is the most commonly used Electron Transport Material (ETM) in PSCs, but its deposition requires a high temperature, which limits its flexibility for commercialization [11].

Zinc oxide (ZnO) has shown some attracted properties that made it as an alternative, such as high electron mobility of 115-155 $cm^2V^{-1}s^{-1}$, stability against photo-corrosion, large excitation binding energy (60 eV) and band gap near the one of TiO_2.

In PSCs, the thickness of the absorber layer, plays an important role in determining its performance. The absorber layer is the central part of PSCs. Many studies have demonstrated that the *PCE* of PSCs is generally dependent on thickness of the perovskite absorber [12, 13].

Perovskite thickness decides charge collection efficiency, fill factor, series resistance and overall *PCE* [12, 13]. When perovskite layer is too thick (> 750 nm), the hole collection will be poor due to an increase in series resistance and recombination within the perovskite layer.

Also, when the absorber layer is thin (say 100 nm), a low photo current is produced which can be seen to arise from poor photon absorption. Therefore, it is important to study and know the appropriate thickness for perovskite absorber in PSCs.

In this study, the role of absorber thickness on solar parameters was investigated using SCAPS. Its influence on the parameters (*PCE*, *FF*, J_{sc}, V_{oc}) was obtained based on the configuration of Glass/FTO/ZnO/$MASnI_3$/CuI/Pt with the aim of obtaining a baseline for device optimization. Here, the simulation was done by varying the thickness from 0.1 µm to 1.3 µm while maintaining all the other device parameters as given in tables 1 and 2.

2 Device Structure and Simulation

The simulation platform provides a powerful tool to have a better understanding about the optical and electrical properties of the solar cell. The Solar Cell Capacitance Simulator (SCAPS-1D) was used to carry out the simulation. The SCAPs was designed to work based on two basic semiconductor equations, which include, the Poisson equation and the continuity equation of electrons and holes under steady-state condition.

The Gaussian energy distribution with a characteristic energy of 0.1 eV was considered as defect states all through the simulation procedure. The thermal velocity of the electrons and holes of 1×10^7 cm/s were taken during the simulation. This simulation software was used to investigate the different performance metrics (Fill factor, short-circuit current density, open-circuit voltage, efficiency) of a perovskite based solar cell.

Tables 1 and 2 summarized the material parameters that were used in this simulation [5, 10-12, 14]. One defect interface is inserted for carrier recombination. The interface defect layer (IDL) is introduced in the ZnO/$CH_3NH_3SnI_3$ interface.

The work functions of the front contact and back contact are 4.40 eV and 5.93 eV respectively [14, 15]. A working temperature of 300 K, solar spectrum AM1.5 of 100 $mWcm^{-2}$ and a scanning voltage of 0-1.3 V were used for all simulations.

Table 1: Defect parameters of interfaces and absorber [10-12,14]

Parameters	**$CH_3NH_3SnI_3$**	**ZnO/$CH_3NH_3SnI_3$ interface**	**$CH_3NH_3SnI_3$/CuI interface**
Defect type	Neutral	Neutral	Neutral
Capture cross section for electrons (cm^2)	2×10^{-14}	2×10^{-14}	2×10^{-13}
Capture cross section for holes (cm^2)	2×10^{-14}	2×10^{-14}	2×10^{-13}
Energetic distribution	Gaussian	Single	Single
Energy level with respect to eV (eV)	0.500	0.650	0.650
Characteristic energy (eV)	0.1	0.1	0.1
Total density (cm^{-3})	1×10^{15}–1×10^{19}	1×10^{17}	1×10^{18}

Table 2: Simulation parameters of PSCs devices [5, 10-12, 14

Parameters	FTO	ETM	Absorber	HTM (CuI)
Thickness (μm)	0.4	0.055	0.45	0.10
Band gap energy E_g (eV)	3.5	3.3	1.30	2.98
Electron affinity χ (eV)	4.0	4.0	4.20	2.10
Relative permittivity ϵ_r	9	9.0	10	6.50
Effective conduction band density N_c (cm^{-3})	2.0×10^{18}	3.6×10^{21}	2.2×10^{18}	2.8×10^{19}
Effective valance band density N_v (cm^{-3})	2.2×10^{18}	1.9×10^{18}	2.2×10^{18}	1.0×10^{19}
Electron mobility μ_n ($cm^2V^{-1}s^{-1}$)	20	100	1.6	1.69×10^{-4}
Hole mobility μ_p ($cm^2V^{-1}s^{-1}$)	10	25	1.6	1.69×10^{-4}
Donor concentration N_D (cm^{-3})	1×10^{19}	1×10^{19}	0	0
Acceptor concentration N_A (cm^{-3})	0	0	1×10^{13}	1×10^{18}
Defect density N_t (cm^{-3})	1×10^{15}	1×10^{13}-1×10^{15}	2.5×10^{13}	1×10^{15}

3 Results and Discussions

3.1 Structure of the simulated PSC and the energy level diagram of the lead-free PSC device

After the simulation, the modeled device alongside its band gap structure is as shown in figures 1a and b. The obtained interface conduction and valence band offset at the $ZnO/CH_3NH_3SnI_3$ interface are 0.28 eV and 2.01 eV while at the $CH_3NH_3SnI_3$/CuI interface, the interface conduction and valence band offset are 1.75 eV and 0.38 eV. In order to avoid recombination and quenching losses from charge carriers, these values are considered beneficial.

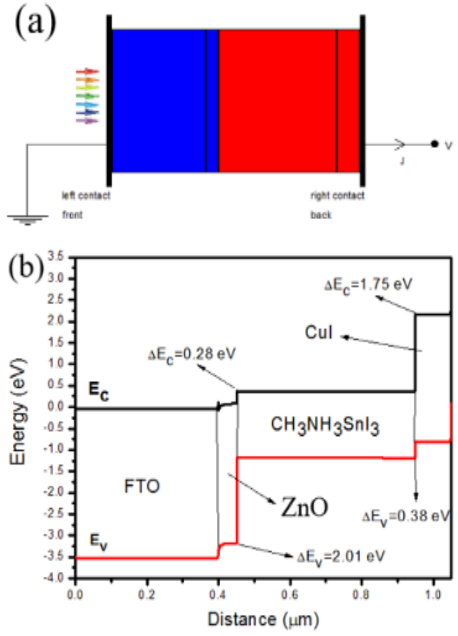


Figure 1: a) The structure of perovskite solar cell in the simulation and b) Energy band diagram of $ZnO/CH_3NH_3SnI_3$/CuI PSC device

The value of conduction band offset prevents the flow of electron charge carrier from the electron transport layer to perovskite layer to the Pt metal contact for minimal recombination. While the large value of the valence band offset denies the flow of holes to the platinum-back contact to prevent their recombination with the electrons in the perovskite layer.

These values are highly crucial in PSCs due to the fact that they encouraged collection of charge carriers which results to higher photovoltaic performance in PSCs. As such, from the result of the band gap structure, ZnO, $CH_3NH_3SnI_3$ and CuI can form a junction when combined to be applied in photovoltaics.

3.2 Performance study of the initial simulation

The Current-Voltage (*J-V*) characteristics of the reference PSC device under illumination is shown in figure 2(a).

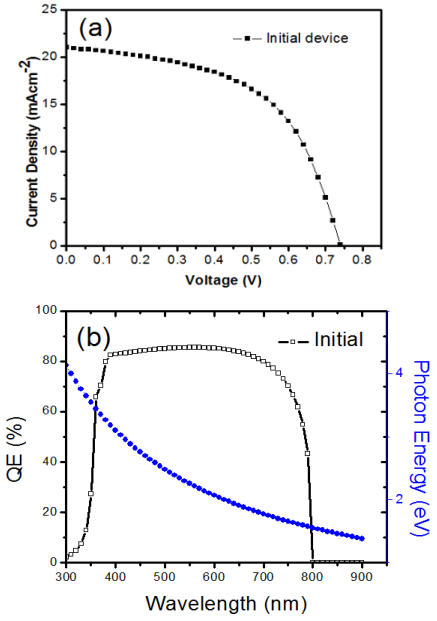


Figure 2: a) J-V curve of PSC with initial parameters and b) quantum efficiency and photon energy of the simulated device with respect to wavelength

Under illumination, a J_{sc} of 20.991 mAcm^{-2}, V_{oc} of 0.741 V, *FF* of 54.048%, and *PCE* of 8.256% were obtained.

When compared with experimental work demonstrated by a group of researchers [16, 17], a comparable V_{oc} (0.85 V) was obtained. To an extent, the values of *PCE*, *FF* and J_{sc} in our simulation are higher than the obtained values from their experimental research work. This could be connected to the additional series resistance arising from Pt metal contact or FTO [15].

Figure 2b shows the quantum efficiency of the device within the range of 300 to 900 nm, which has maximum attained value of 90% observed at 550 nm. Optical absorption edge is red shifted to 800 nm which corresponds to a band gap of 1.30 eV in $CH_3NH_3SnI_3$.

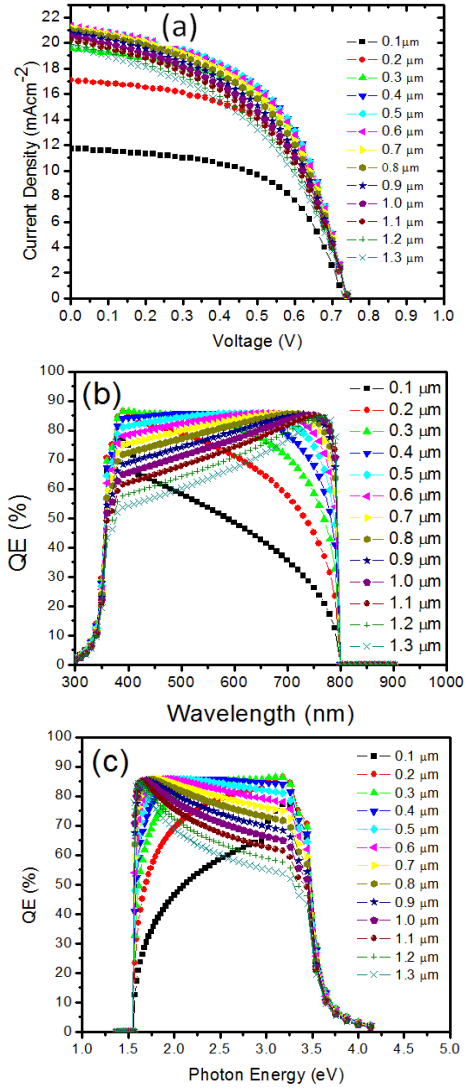


Figure 3: a) J-V curves of PSC with varied absorber thickness, b) quantum efficiency vs wavelength of PSC with varied absorber thickness and c) quantum efficiency vs Photon energy of PSC with varied absorber thickness

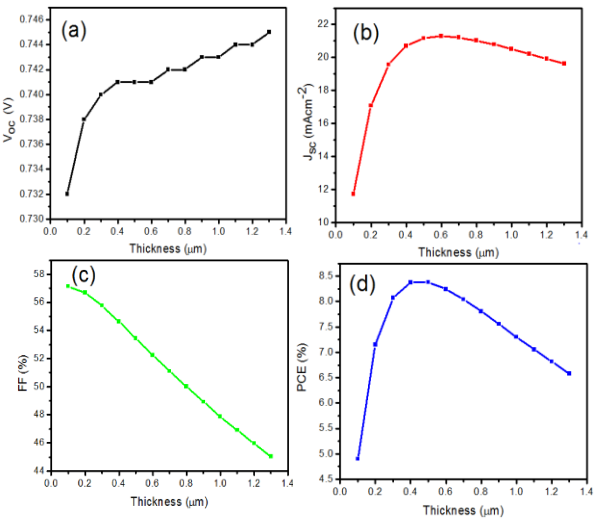


Figure 4: Variation in solar cell parameters with increasing absorber layer thickness

3.3 *Effect of thickness of absorber layer*

The thickness of the absorber layer is one of the important parameters contributing to optimizing solar cell performance. It is therefore very important to make good choice for absorber thickness in order to determine device's performance. The *J-V* and QE of the varied absorber thickness is shown in figures 3(a), (b) & (c). The influence of thickness of absorber on different solar cell parameter metrics; V_{oc}, J_{sc}, *FF* and *PCE* is depicted in figures 4(a-d).

From our simulation study, *PCE* is lower when thickness of the layer is too small which can be ascribed to the poor light absorption by the material. For thicknesses beyond 0.5 µm, the collection of generated carriers decreased because of charge recombination [14].

There was a steady increase in *PCE* with increase in layer thickness from 0.1 to 0.5 µm which is due to the production of new charge carriers while the steady decrease from 0.6 µm to 1.3 µm is due to lesser electron and hole pairs extraction rate that leads to recombination process.

As shown in Figure 3(a), J_{sc} increases from 11.717 to 21.284 mAcm^{-2} with thickness increase from 0.1 to 0.6 µm. This increase is due to the increase in carrier generation and dissociation in the absorber layer [18, 19].

After 0.6 µm, the J_{sc} then starts decreasing from 0.7 to 1.3 µm. Fill factor decreases slightly with thickness increase in the perovskite layer. The decrease is attributed to the high recombination of generated charge carriers at the perovskite layer [15, 20]. Table 3 shows the photovoltaic parameters obtained during the simulation.

Table 3: J-V characteristic parameters with the variation of thickness of absorber

Parameters T (μm)	J_{sc} (mAcm^{-2})	V_{oc} (V)	*FF* (%)	*PCE* (%)
0.1	11.717	0.732	57.141	4.899
0.2	17.085	0.738	56.679	7.149
0.3	19.566	0.740	55.768	8.073
0.4	20.700	0.741	54.646	8.377
0.5	21.166	0.741	53.439	8.382
0.6	21.284	0.741	52.240	8.244
0.7	21.212	0.742	51.110	8.043
0.8	21.034	0.742	50.004	7.807
0.9	20.795	0.743	48.924	7.556
1.0	20.523	0.743	47.870	7.301
1.1	20.231	0.744	46.901	7.056
1.2	19.930	0.744	45.962	6.816
1.3	19.624	0.744	45.037	6.580

Figures 3(b) and (c) show the QE as a function of wavelength and also function of photon energy with varied $CH_3NH_3SnI_3$ layer thickness at wavelength range of 300 nm to 900 nm. The QE first increases rapidly with the $CH_3NH_3SnI_3$ thickness from 0.1 μm to 0.5 μm and decreases slightly after the thickness is greater than 0.5 μm, which shows that 0.5 μm thickness of $CH_3NH_3SnI_3$ layer can absorb most of the incident photons and the part beyond 0.5 μm can only contribute little to the PSC performance [18, 19].

Therefore, the optimized perovskite absorber layer thickness is around 0.5 μm which gives V_{oc} of 0.741 V, J_{sc} of 21.166 mAcm^{-2}, *FF* of 53.439 % and *PCE* of 8.382%. There was also a decrease in V_{oc} with decreasing thickness. The decrease in V_{oc} is attributed to the increment in the dark saturation current, which increases the recombination of the charge carriers when the thickness is small.

This can be explained by the dependency of open-circuit voltage on the photo-generated current and dark saturation current, which is written as in equation (1) [12, 21]:

$$V_{OC} = \frac{kT}{q}\ln\left[\frac{J_{SC}}{J_O}+1\right] \quad (1)$$

Where kT/q is the thermal voltage, J_{sc} is the photo-generated current density, and J_o is the saturation current density. Figure 4(a-d) shows variation of V_{oc}, J_{sc}, *FF* and *PCE*, with absorber thicknesses (from 0.1-1.3 μm). The optimum *PCE* was obtained at thickness value of 0.5 μm. As shown, it is evident that proper absorber layer selection with suitable thickness can reduce quenching losses in PSCs.

4 Conclusion

In this paper, the numerical simulation of Tin based perovskite solar cell was performed using SCAPS-1D simulation software. The absorber thickness was varied from 0.1 μm to 1.3 μm. The results revealed that the optimal $MASnI_3$ thickness was 0.5 μm, which gave *PCE* of 8.382%, J_{sc} of 21.166 mAcm^{-2}, V_{oc} of 0.741 V and *FF* of 53.439 %. When the optimized result is compared with the initial device, an improvement of ~ 1.02 times in *PCE*, ~ 1.01 in J_{sc} was obtained over the device reference. The findings show that $CH_3NH_3SnI_3$ is an alternative absorber to the lead-based perovskite absorber.

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Declaration of Competing Interest

Authors have declared that there was no conflict of interest.

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