Simulation of a perovskite sandwich solar cell with the p-CZTS / p-CH$_3$NH$_3$PbCl$_3$ / p-CZTS absorber layers

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Abstract. Perovskite solar cells attract the attention because of their unique properties in photovoltaic cells. Numerical simulation to the structure of Perovskite on p-CZTS/p-CH$_3$NH$_3$PbCl$_3$/p-CZTS absorber layers is performed by using a program solar cell capacitance simulator (SCAPS-1D), with changing absorber layer thickness. The effect of thickness p-CZTS/p-CH$_3$NH$_3$PbCl$_3$/p-CZTS, layers at (3.2μm, 1.8 μm, 1.1 μm) respectively are studied. The obtained results are short circuit current density ($J_{sc}$), open circuit voltage ($V_{oc}$), fill factor (F.F) and power conversion efficiency (PCE) equal to (28 mΑ/cm$^2$, 0.83 v, 60.58 % and 14.25 %) respectively at 1.1 μm thickness. Our findings revealed that the dependence of current - voltage characteristics on the thickness of the absorbing layers, an increase in the amount of short circuit current density with an increase in the thickness of the absorption layers and thus led to an increase in the conversion efficiency and improvement of the cell by increasing the thickness of the absorption layers.

1. Introduction
In the past decades. Several articles have been published in the development of perovskite solar cell PSC, using different techniques under multiple parameters, in addition to practical fabrication, there are many numerical simulations to simulate proposed structure. Numerical simulation have been mad using SCAPS by Kojima et.al 2009 [1] the perovskite solar cells was two organolead halide, power conversion efficiency PCE was 3.8 %. Tin Halide perovskite solar cells studied by B.J.Babu et.al using SCAPS-1D 2018 [2], the power conversion efficiency PCE was 25.91 %. The absorber layers in the previous studies was highly toxic. Our study aimed to improve such kind of solar cell by changing the absorber layers thickness with low toxicity. (p-CZTS/p-CH$_3$NH$_3$PbCl$_3$/p-CZTS) absorber layers with different thickness (3.2 μm, 1.8 μm and 1.1 μm) respectively. For perovskite solar have been simulated using SCAPS Method. Perovskite solar cell sandwiched (PSCs) advantages are high absorption coefficient and easy fabrications. These advantages make them very attractive for future solar cell technologies. The PCE obtained was 14.25 %. The advantages of changing absorber layer thickness leads to efficient solar cells.

2. Numerical simulation
Basic semiconductor equations simulation by SCAPS-1D Computer-based window application, Possion and continuity equation [3]. Thus, is used in this study to simulate PSCs and study properties (I–V) [4], as given in equation (1).
\[ \text{V}_{\text{oc}} = \frac{k_t}{q} \ln \left( \frac{j_{sc}}{j_0} + 1 \right) \]  

(1)

Where \( k = \) Boltzmann constant, \( t = \) Operating Temperature, \( j_0 = \) Reverse saturation current, \( q = \) Electron charge. The parameters set for simulation are selected from the previous experimental work Ismaila.B, et.al to study the hole transporting material effect on perovskite based solar cells using SCAPS – 1D [5-6]. Table 1 summarizes all the parameters in the simulation process.

![Figure 1. Architecture of simulated model.](image)

**Table 1.** The parameters set based at (300°k) and AM1.5sun.

| Layers | FTO | ZnO | CZTS | CH\(_3\)NH\(_3\)PbCl\(_3\) | HTM |
|--------|-----|-----|------|-----------------|-----|
| Thickness, x (\(\mu m\)) | 0.5 | 0.05 | 0.25 | 0.5 | 0.35 |
| Band gap, \(E_g\) (eV) | 3.5 | 3.35 | 1.55 | 1.55 | 2.45 |
| Electron affinity, \(x\) (eV) | 4 | 4.21 | 4.5 | 3.9 | 3 |
| Dielectric permittivity, \(\varepsilon/\varepsilon_0\) | 9 | 9E0 | 10 | 6.5 | 3 |
| \(N_e\) (\(cm^{-3}\)) | 2.2E+18 | 2.2E+18 | 2.2E+18 | 2.2E+18 | 1E+15 |
| \(N_H\) (\(cm^{-3}\)) | 1.8E+19 | 1.8E+19 | 1.8E+19 | 1.8E+19 | 1E+19 |
| Electron thermal velocity (\(cm/s\)) | 2E+1 | 2.5E+1 | 1E+2 | 1.6E0 | 2E-4 |
| Hole thermal velocity (\(cm/s\)) | 1E0 | 1E+2 | 2E+1 | 2E-1 | 2E-4 |
| Electron mobility (\(cm^2/v.s\)) | 1E+7 | 1E+7 | 1E+2 | 3E+7 | 1E+7 |
| Hole mobility (\(cm^2/v.s\)) | 1E+7 | 1E+7 | 1E+7 | 3E+7 | 1E+7 |
| \(N_D\) (\(cm^{-3}\)) | 2E+19 | 1E+18 | 0E0 | 0E0 | 0E0 |
| \(N_A\) (\(cm^{-3}\)) | 0E0 | 0E0 | 8.22E+18 | 6E+18 | 2E+18 |
| Reference | [7] | [8] | [9] | [10,11,12] | [13] |

3. Results and discussion

The study is done on the structure of the perovskite solar cell sandwiched FTO/n-Zn O/p-CZTS/p-CH\(_3\)NH\(_3\)PbCl\(_3\)/p-CZTS/HTM, these layers include HTM hole transport material, Zn O buffer, and FTO window, as shown in figure 1. The incident photons will interact with the absorber layer resulting in photo-exited carriers. Based on the fact the depending of photo generated carriers on the thickness of the absorber layer, the absorber layer thickness has been changed to an optimum thickness to obtain more efficient solar cell. Modification of absorber layer thickness clearly affected the
diffusion length of carriers, very thin absorber layer will decrease the absorption rate. The optical absorption in addition of photo generated carriers depending on the length of diffusion which are directly proportional with the width of the absorber layer. The dependence of solar cell parameters such as PCE, F.F, $J_{sc}$, $V_{oc}$ with varying thickness are shown in figure 2.

![Figure 2. The first absorber layer (p-CZTS).](image)

Based on figure 2, the $V_{oc}$ is increasing slightly with the increasing of thickness. In this figure, the first absorber layer (p-CZTS) PCE of 13% with $J_{sc} = 24.58$ mA/cm², $V_{oc} = 0.8$ v, and F.F = 66.53 %. This is achieved when the thickness reaches (3.2 μm). When the thickness is increasing from (1 μm) to (3.2 μm), both of PCE and, $J_{sc}$ increase up to (3.2 μm). This represents the increase in the generation of the electron and hole pairs in the absorber layer. But when it increases from (1 μm) to higher amount, the PCE and, $J_{sc}$ both undergo saturation. This indicates the recombination of charges inside the absorber layer before reaching the contacts.

![Figure 3. The second absorber layer (p- CH₃NH₃PbCl₃).](image)
In this layer, PCE is(14%), with, $J_{sc} = 25.98 \text{ mA/cm}^2$, $V_{oc} = 0.83 \text{ v}$, and $F.F= 64.24 \%$. This is achieved when the thickness reaches (1.8 $\mu$m). In this case, when the thickness increases from (0.6 $\mu$m) to (1.8 $\mu$m), both of PCE and, $J_{sc}$ increase up to (1.8 $\mu$m).

![Figure 4. The third absorber layer (p-CZTS)](image)

In this layer, PCE is 14.25% with, $J_{sc} = 28 \text{ mA/cm}^2$, $V_{oc} = 0.83 \text{ v}$, and $F.F= 60.58 \%$. When the thickness increases from (0.1 $\mu$m) to (1.1 $\mu$m), the PCE and, $J_{sc}$ also increase up to (1.1 $\mu$m). The thickness of first absorber layer (p-CZTS) was changed from (1 $\mu$m) to (3.2 $\mu$m); the second layer (p-CH3NH3PbCl3) from (0.6 $\mu$m) to (1.8 $\mu$m) and the third layer (p-CZTS) from (0.1 $\mu$m) to (1.1 $\mu$m). To reach a higher performance level, the architecture of perovskite solar cell should have significant characteristics like use less harmful materials and easy fabrication, and low cost.

4. Conclusion

Using simulation program SCAPS-1D. The changes done thickness layers of the three absorption for the first (p-CZTS), second (p-CH3NH3PbCl3) and third (p-CZTS) layers as follows (1-3.2) $\mu$m, (0.6 - 1.8) $\mu$m, (0.1-1.1) $\mu$m, respectively. Hence, the high-performance of a solar cell is achieved at the thickness of (1.1 $\mu$m). When the absorption layer defects are reduced, the performance of the solar cell improves, and we find through simulation that a layer CH3NH3PbCl3 layer attained (14%) for PCE. By simulating the model, the absorption layers thickness influences perovskite solar cell to achieve higher efficiency. The results show that the maximum rates attained for PCE, $J_{sc}$, $F.F$ and $V_{oc}$ were (14.25%, 28 mA/cm$^2$, 60.58 %, and 0.83 v), respectively.

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5. Reference

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