The influence of the interface layer between the electron transport layer and absorber on the performance of perovskite solar cells

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Abstract. High efficiency, lightweight, and cost-effectiveness put the perovskite solar cells to the top of the focus researches of solar cells. The architecture of the cell especially the energy band alignment at the interface is a critical issue in the cell performance. In the current paper, the solar cell structure under investigation consists of TiO2, CH3NH3PbI3, and Spiro OMe TAD as electron transport layer, absorber and hole transport layer respectively. A 3C-SiC material with energy gap of 2.420 eV was used as interface layer. The role of the interface layer between the perovskite and electron transport layer was considered. Before inserting the interface layer, a parametric study including the thickness and doping of each layer, was achieved. The results showed that the best performance of the cell at a thickness of 400 nm, 300 nm, 200 nm for absorber layer, ETL, and HTL respectively, with a doping concentration of 1014 cm−3, 1019 cm−3, 1019 cm−3 for the same layers. These parameters give a Voc, Jsc, FF, and PCE of 1.11 V, 28.9 mA∙cm−2, 83.19%, and 26.88% respectively. Inserting an interface layer improved the performance of the cell where the PCE increased over 29% at a thickness of 90 nm. The results showed that the parameters of the interface layer play a significant role in cell performance.

1. Introduction

The endless expansion in world population and improved lifestyle continuously brings up a larger demand for electricity to power produces. With global warming being a major climate issue worldwide, the use of renewable energy could represent a valuable alternative to help to reduce the effect of pollution, which is the main drawback of conventional power generating devices. Natural sources like water and wind are still recruited in electrical power generation. However, the sun is still one of our greatest sources of energy, which could be utilized through the introduction of solar cells. The latter’s mode of action is usually based on the conversion of light or photons into electricity; for that reason, it is often referred to as a photovoltaic device [1].

The perovskite solar cells (PSCs) are the most recent photovoltaic devices which use the light-absorbing layer made of perovskite material. A long carrier diffusion length, high light absorption, and tunable bandgap are the main features that made perovskite solar preferable over the conventional solar cells [2]. Since their introduction, they have dragged considerable attention due to their high efficiency (>15%) and remarkable ease of processing over large areas [3]. PSC is composed of organic metal halide as an absorber. The lead halide perovskite
material is promising to use in the production of perovskite solar cells due to its superior optoelectronic properties [4].

In addition to the cathode and anode, the PSC comprises three main layers which are the hole transporting material layer (HTL), the absorber perovskite layer, an electron transporting material layer (ETL). From their names, the function of the HTL is to extract and transfer holes and block electrons while the function of ETL is to block the holes and transfer the electrons [5]. Upon absorption of light, photo-generation of free charge carriers occurs in the absorber, and these carriers, under the built-in potential will drift to HTL-perovskite and ETL-perovskite interface region. The weak charge transport and/or the energy barrier of the HTL or ETL will produce the charges accumulation at the border of the interface of these layers and this will cause an increase in charges recombination and hence reduce the solar cell efficiency. Therefore, to avoid the aforementioned problem, the interfacial materials should be engineered carefully. In the present work, a layer of n-3C-SiC was added as an interface layer between ETL and the perovskite layer. The added layer would hopefully improve the charge transfer between the layers due to band match and decreases the energy losses of the electrons during transportation which in turn lead to enhance the photovoltaic performance.

2. Simulation details
In the present work, the perovskite solar cell simulation was achieved using SACPS (Solar Cell Capacitance Simulator). SCAPS is a 1D simulation program with a multi-layers (up to seven) input. This software was developed by a group at the Department of Electronics and Information System, University of Gent, Belgium [6]. To simulate the proposed device, the individual parameters for each layer should be well defined. In terms of the energy bandgap ($E_g$), electron affinity ($\chi$), dielectric permittivity ($\epsilon$), conduction and valence band density of states ($N_C$ and $N_V$), electron and hole mobility ($\mu_e$ and $\mu_h$), and donor and acceptor density ($N_D$ and $N_A$), the property of each layer were used as an input to the simulator. These parameters were taken from the literature [4,7-9] and are summarized in Table 1.

| Parameters                                      | TiO$_2$ | n-3C-SiC | CH$_3$NH$_3$PbI$_3$ | Spiro OMe TAD |
|------------------------------------------------|--------|----------|--------------------|--------------|
| Bandgap $E_g$ (eV)                              | 3.2    | 2.420    | 1.55               | 3.0          |
| Electron affinity (eV)                         | 4.0    | 3.830    | 3.9                | 2.45         |
| Dielectric permittivity                        | 9.0    | 9.720    | 10.0               | 3.0          |
| CB effective density of states (1/cm$^3$)      | 2×10$^{18}$ | 1.553×10$^{19}$ | 2×10$^{18}$ | 2.2×10$^{18}$ |
| VB effective density of states (1/cm$^3$)      | 2×10$^{19}$ | 1.163×10$^{19}$ | 2×10$^{19}$ | 1.9×10$^{19}$ |
| Thermal velocity of electron (cm/s)            | 10$^7$ | 1×10$^7$ | 10$^7$             | 10$^7$       |
| Thermal velocity of hole (cm/s)                | 10$^7$ | 1×10$^7$ | 10$^7$             | 10$^7$       |
| Electron mobility (cm$^2$/Vs)                  | 0.2    | 650      | 1.0                | 2.0×10$^{-4}$ |
| Hole mobility (cm$^2$/Vs)                      | 0.1    | 40       | 1.0                | 2.0×10$^{-4}$ |
| Shallow uniform donor density $N_D$ (1/cm$^3$)  | 10$^{19}$ | 10$^{18}$ | 10$^{14}$         | –            |
| Shallow uniform acceptor density $N_A$ (1/cm$^3$)| –      | –        | –                  | 10$^{19}$    |

As shown ‘in Figure 1’, the current device having a structure of TiO$_2$, CH$_3$NH$_3$PbI$_3$, and Spiro OMe TAD as ETL, absorber, and HTL respectively. The initial values of thickness and doping for each layer are given in Table 2 [4]. The thickness and doping concentration were changed to obtain the solar cell structure with the best performance. A thin layer of 3C-SiC was inserted in the optimum structure between ETL and absorber as an interface layer. The standard conditions, illuminated under AM1.5G solar spectrum with 100 mW.cm$^{-2}$ incident power
density and temperature of 300 °K, are considered in the current study. The absorption coefficient of the absorber, HTL, and ETL are defined in the program for simulation.

Table 2. Initial values of thickness and doping of the proposed cell.

| Layer | Thickness (nm) | Doping (cm⁻³) |
|-------|----------------|---------------|
| Absorber | 200            | 10¹¹          |
| HTL    | 700            | 10¹⁸          |
| ETL    | 100            | 3×10¹⁹        |

3. Results and discussion

To obtain the optimum structure of the solar cell that gives the best performance the current study involved two main parts, the first is the optimum thickness and doping density of each layer of the cell while the second part focused on the role of the interface layer between the perovskite and ETL on the cell parameters.

3.1 Effect of layers thickness

To obtain best absorption of the solar light in the perovskite layer and hence increase the generation process of electron-hole pairs the thickness of the absorber layer has been varied from 100 nm to 900 nm. Figure 2 illustrated the variation of the solar cell parameters with the absorber layer thickness. As shown in Figure 2 the Jₛₑ increased from 19.88 mA·cm⁻² to 43.61 mA·cm⁻² over the examined thickness range, while Vₒc slightly decreases from 1.18 V to 1.08 V. The absorber thickness effect noticeably on the efficiency although the FF drop from 84.5% to 75.98%. As represented in figure 2 the cell efficiency increased from 20% to 36%. This increase can be signed to the photo absorption enhancement in this layer. This means that the number of photo-generated carriers is associated with the total amount of absorbed photons, resulting in a Jₛₑ increase with layer thickness increases. It can be noticed that above 300 nm the increase in Jₛₑ trend to be slow compare to the Jₛₑ variation at low absorber thickness. The efficiency has the same behavior in this range. This could be ascribed to the saturation in the light absorption occurs. As the absorber becomes thicker, the photo-generated carriers at the center of the absorber layer will recombine when the thickness of this layer exceeds the diffusion length. This is reflected on the Vₒc due to the decrease in the effective band gap, also, to increase in the recombination processes [9-12]. Although the maximum efficiency was found to be 36% at absorber thickness of 900 nm the results show that the better thickness of 400 nm

![Figure 1. Perovskite solar cell structure.](image-url)
where the efficiency significantly improved to 31% with $J_{sc}$, $V_{oc}$, FF of 33 mA·cm$^{-2}$, 1.12 V, and 83%, respectively.

Figure 2. The variation of solar cell parameters with absorber thickness.

‘Figure 3.’ illustrates the thickness influence of the electron transport layer on $J_{sc}$, $V_{oc}$, FF, and PCE. This figure reveals a dramatic decrease in the $J_{sc}$ and PCE with increasing the electron transport layer thickness while no significant influence of the thickness increasing on the $V_{oc}$ and FF. As shown in figure 3 the $J_{sc}$ decreases from 33.2 mA·cm$^{-2}$ to 10.29 mA·cm$^{-2}$ and PCE decreases from 31% to 9.1% over the ETL thickness from 100 nm to 1000 nm. The impact of the electron transport layer on the solar cell parameters can be attributed to the fact that the TiO$_2$ has a critical drawback of intrinsic low mobility and increasing the thickness of this layer will result in a charge accumulation and hence increases the recombination. The best performance was found at a thickness of 300 nm [4].

Figure 3. The variation of solar cell parameters with ETL thickness.

Keeping the thickness of the absorber and ETL at the optimum thicknesses which gave the best cell performance, the effect of the HTL thickness on the cell performance was also studied by varying the thickness of this layer over the range from 100 nm to 1000 nm with step of 200 nm. ‘Figure 4’ shows that the thickness of HTL does not have a critical impact on the solar cell performance and the values of $V_{oc}$, $J_{sc}$, FF, and PCE are around 1.12 V, 33.27 mA·cm$^{-2}$, 83.25%, and 31% respectively. This result agrees with what was obtained by Hima et. al., and it can be
attributed to the constant number of charge carriers produced in the absorber layer [4]. We used a 200 nm as a reference thickness for this layer.

![Figure 4](image1.png)

**Figure 4.** The variation of solar cell parameters with HTL thickness.

### 3.2 Effect of layers doping

Layer doping plays a critical issue in decides the electrical behavior and hence the performance of the solar cell. To improve the cell performance proper doping of ETL, HTL and absorber are necessary. The impact of the doping concentration of the absorber layer was investigated by varying the doping level from $10^{12}$ cm$^{-3}$ to $10^{22}$ cm$^{-3}$. 'Figure 5' shows the change in cell parameters with doping density, it can be seen that the cell parameters are almost unchanged with increasing the absorber density until the doping concentration of $10^{17}$ cm$^{-3}$. Above the doping level of $10^{17}$ cm$^{-3}$, a dramatic decrease in the $J_{sc}$, FF, and PCE was observed while an increase in the $V_{oc}$ from 1.18 V to 2.6 V can be noticed. The reason which stands behind this behavior is that high doping leads to a reduction in the width of the depletion region and hence increases the recombination process at the bulk of the absorber [13]. The current results show that doping density for the absorber layer ($>10^{16}$ cm$^{-3}$) is not suitable for high efficiency.

![Figure 5](image2.png)

**Figure 5.** The variation of solar cell parameters with absorber doping.

The HTL doping impact on solar cell performance was studied by varying the acceptor concentration from $10^{17}$ cm$^{-3}$ to $10^{22}$ cm$^{-3}$. As shown 'in Figure 6’ the difference overdoping
concentration are FF and PCE while both $J_{sc}$ and $V_{oc}$ are almost constant and independent of acceptor concentration which indicates that the recombination rate is unrestrained of doping density. The recombination rate affects minority carrier’s density and at high doping of acceptor in HTL the density of minority deceases which in turn blocks the electrons from absorber [14]. A dramatic increase in the FF and PCE at doping density above $10^{18}$ cm$^{-3}$ could be attributed to the sheet resistance and conductivity enhancement in HTL at a high doping rate [15]. Doping over $10^{18}$ cm$^{-3}$ gives a best cell performance with efficiency of 25.3 %.

By keeping the doping density of perovskite and HTL at $10^{14}$ cm$^{-3}$ and $10^{19}$ cm$^{-3}$ respectively the doping concentration of ETL was varied from $10^{17}$ cm$^{-3}$ to $10^{22}$ cm$^{-3}$ to investigate the impact of the ETL doping on the solar cell performance. ‘Figure 7’ shows that the cell parameters remain unaffected by donor doping variation and this can be attributed to the Moss-Burstein effect [16]. The results of the doping rate in the ETL suggest that ETL doping density at $10^{19}$ cm$^{-3}$ is the better value for best cell performance.

From the aforementioned parametric study of the thickness and doping of each layer, one can conclude the optimum structure parameters are 400 nm, 200 nm, 300 nm as a thickness of
absorber layer, HTL, and ETL respectively, while the doping of $10^{14}$ cm$^{-3}$, $10^{19}$ cm$^{-3}$, $10^{19}$ cm$^{-3}$ for the same layers. These parameters give a $V_{oc}$, $J_{sc}$, FF, and PCE of 1.11 V, 28.9 mA cm$^{-2}$, 83.19%, and 26.88% respectively.

3.3 Interface layer:
To boost the PCE, the charge losses at the interface between the perovskite/ETL and/or perovskite/HTL should be reduced. One of the interface engineering strategies is to use a thin layer between the active layer and HTLs (ETLs) to improve the energy alignment and hence the charge transport across the interfaces. In the current study, the interface layer of 3C-SiC was used in the optimum structure between ETL and absorber. To study the impact of this layer on the cell parameters the thickness and doping density were taken into consideration. The thickness was varied from 30 nm to 100 nm, with doping density of $10^{16}$ cm$^{-3}$, and the results are presented in Figure 8. It can be seen that the $J_{sc}$ increases slightly from 29.6 mA cm$^{-2}$ to 31.5 mA cm$^{-2}$ and this can be ascribed to the reduction in the charge recombination. The interface layer makes a drop of energy barrier at the perovskite/interfacial layers which in turn facilitates the charge transfer. This explanation enhances the stability in $V_{oc}$ over the examined interface thickness. An enhancement in the PCE from 27.6% to 29% was also noticed.

Figure 8. The variation of solar cell parameters with interface thickness.

To study the impact the doping of interface layer on the cell performance the donor doping density of this layer was varied from $10^2$ cm$^{-3}$ to $10^{18}$ cm$^{-3}$. The results show that the doping density does not affect significantly on the cell parameter until doping density of $>10^{15}$ cm$^{-3}$ and beyond this value of doping the $J_{sc}$ decreases slightly while an increase in the PCE from 28.8% to 29.25% due to narrowing the depletion region beneficial for charge carrier collection.
4. Conclusions

In the present work, the impact of layer thicknesses and doping of CH$_3$NH$_3$PbI$_3$-based solar cell on different electrical parameters was investigated. It was found that the perovskite layer thickness has a significant influence on electrical parameters in comparison with that of HTL and ETL. It was found that the optimized layer thickness values were 400 nm, 200 nm, and 300 nm for the perovskite layer, HTL, and ETL, respectively which provided the better power conversion efficiency of 26.88%. The parametric study of the doping variation on the proposed structure showed that the doping density for absorber layer (> 10$^{16}$ cm$^{-3}$) was not suitable to obtain a high efficiency while the doping of acceptor in HTL (> 10$^{16}$ cm$^{-3}$) enhanced the cell performance whilst the cell parameters remained unaffected by ETL donor doping variation.

With regards the interface layer, the present work demonstrated that the introduction of n-3C-SiC into the solar cell design evidently had a good effect on enhancing the overall cell performance through achieving an enhancement in efficiency by improving charge transport and reducing recombination; which was in correspondence to the proposed hypothesis. Within the tested thickness range, it was shown that the lower the thickness, the better the device efficiency obtained. In contrast, it was found that the highest doping density within the used range produced the best observed improvement in device efficiency. However, it is worth to consider that these findings need to be further investigated using other interface materials rather than n-3C-SiC to confirm the current findings. This in turn can uncover additional possibilities for future versions of solar cell devices, opening the horizon for an entirely new fields of knowledge and research.

5. References

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