Study of defects in CH$_3$NH$_3$PbI$_3$-based perovskite solar cells

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Abstract. The present work will focus on the investigation of the influence of defects density and carriers capture cross-section are in absorption layer on the performance of perovskite solar cells. Furthermore, the impact of defect density in the electron transport material ETM/absorber interface layer will also be studied. The hybrid halide perovskite solar cells are chosen in this work and will be simulated by using one-dimension solar cells capacitance simulation SCAPS-1D. The proposed structure of the perovskite solar cell is a planar FTO/ETM/ perovskite/ HTM based on TiO$_2$ and Spiro-OMeTAD as electron transport layer ETM and hole transport layer HTM, respectively, and on CH$_3$NH$_3$PbI$_3$ as absorber layer (perovskite). The results showed that when the defect density in the absorber layer was varied from $10^{10}$cm$^{-3}$to $10^{18}$ cm$^{-3}$, the cell parameters, open circuit voltage ($V_{oc}$), the short circuit current ($J_{sc}$), the fill factor (FF), and the efficiency (PCE) were significantly decreased. At high defect density ($10^{18}$ cm$^{-3}$), the defect affects negatively on the cell performance due to the high recombination rate of Shockley Read Hall. Similarly, the capture cross section exhibits similar behaviour in the active layer. By increasing the defect density in the ETM/absorber interface layer, the main cell parameters PCE, FF, and $J_{sc}$ are slightly reduced and there has been no noticeable impact on $V_{oc}$.

1. Introduction

Photovoltaic solar is becoming one of the challenging solutions to the problems of securing a clean and sustainable energy source. This includes Si-based solar power cells and photovoltaic cells that are sensitized as well as the organic solar cells [1]. Recently, inorganic-organic solar cells of the metal halide Perovskite have gained considerable global attention as a candidate for low-cost and high-performance photovoltaic over the last few years. Organ lead halide perovskite materials properties, such as its broad duration of electron-hole diffusion, good electron-hole mobility, and large coefficient of absorption have several advantages for photovoltaic device application [2]. There has been a discovery of the existence of perovskite substances in solar panels with an efficiency (PCE) lower than 4% [3]. In the short time in the history of solar cells, where the newly reported power conversion efficiency is 22.1%, rapid chronological progress is seen [4]. Perovskite, such as methyl ammonium lead iodide (MAPbI$_3$), shows different intrinsic defects caused by vacancies, interstitial, and antisites. Despite its past problem with perovskite is good with defects tolerance, this recent research has demonstrated that deep level defects are present in the Shockley Quiesser (SQ) restricted approach that affects the performance of perovskite solar cell (PSC). Different studies demonstrated the impact of defect density on hybrid Organic-inorganic perovskite (HOJPS) solar cells efficiency [5], however, there is no comprehensive study available yet. To make Perovskite solar cells a winner against traditional technology of solar cells, a deep understanding is thus needed. It is possible to classify the defect based on its location in the band gap energy, where they can be detected at either deep or shallow levels [5]. Si Fengjuan et al. studied the effects of defects in PSC in particular the defect states in the
absorption layer and adjacent interfaces [6]. A.S.Chouhan et al studies to simulate self-consistent system model with SCAPS using data of the experimental from 17.5% efficiency PSC. Experiential results, such as doping consideration of compactness TiO$_2$, densities of the defect and doping in perovskite. The only reasonable variables in the model are the interface layer defect density at the HTM/perovskite and perovskite/ETM. For simulation, it was shown that the HTM interface layer defect density strongly affects the $V_{oc}$, whereas ETM interface layer has a significant influence on $J_{sc}$ [7]. M.S. Jamal et al [8] presented SCAPS-1D's numerical analysis on inverted planer NiO-based PSC as a hole transportation material (HTM) and investigated the impact of the absorption layer and HTM /absorber interface layer's defect density and energy levels on output. The result is obtained when various energy levels of up to 0.9 eV have been studied for different defect density values from $10^{13}$ cm$^{-3}$to$10^{16}$cm$^{-3}$. Deeper defects, less than 0.2eV, and higher defect density were found to produce a low efficiency. The perovskite layer has been examined in regards to its optical and structural characteristics be deficient. Then numerical investigations of the effect of perovskite absorption layer thickness on related solar cell parameters have been done using SCAPS-1D as well as the defect density of the absorption layer. Since the active layer thickness changes from 200-800 nm and shallow level defect changed from $10^{13}$ cm$^{-3}$ to $10^{16}$ cm$^{-3}$, the efficiency reduced sharply from 26.7% to 0.9%. However, the PCE decrease from approximately 19.3% to approximately 6.15% as the thickness and the deep density increase from 200-800 nm and $10^{13}$ cm$^{-3}$ to $10^{16}$ cm$^{-3}$, respectively [9]. Until nowadays, there are not enough studies investigated the effect of defect mechanism in solar perovskite cells. In this paper, the aim is to investigate various aspects of defects in planer PSC structure: Glass/FTO/TiO$_2$/$CH_3NH_3PbI$_3$/Spiro-OMeTAD/ back contact, which is simulated using the 1-D capacitance simulation for solar cells (SCAPS-1D) [10]. The work studies the impact of defects on the PSC performance, where the focus will be on the carriers capture cross-section area, defect density in the absorption layer, and defect density in ETM / perovskite interface layer.

2. Device simulation parameters
SCAPS 1D software is employed in this work as it is considered one of the most effective and user-friendly numerical simulations of solar cell systems. The proposed structure of perovskite solar cell is a planer structure of glass /FTO (Fluorine doped Tin Oxide) /TiO$_2$ (Electron Transportation layer)/$CH_3NH_3PbI$_3(active layer)/Spiro-OMeTAD (Hole Transportation layer)/metal back contact. Figure 1 illustrates the basic structure for the studied solar cell, whereas the values of the simulation parameters are summarized based on values found in the literature as shown in table 1. Table 2 summarizes defects parameters of the absorber layer and interfaces ETM/absorber and HTM/absorber of the perovskite solar cell.

![Figure 1. The basic structure of the perovskite solar cell.](image-url)
Table 1. Simulation parameters of perovskite solar cells devices.

| Parameter                                  | FTO[13] | TiO₂[12] | CH₃NH₃PbI₃[7] | Spiro-OMeTAD[11] |
|--------------------------------------------|---------|----------|----------------|-----------------|
| Thickness \( t \) (µm)                     | 0.4     | 0.001    | 0.4            | 0.4             |
| Band gap \( E_g \) (eV)                    | 3.5     | 3.26     | 1.55           | 3.06            |
| Electron affinity \( \chi \) (eV)          | 4       | 3.7      | 3.9            | 2.05            |
| Dielectric permittivity \( \varepsilon_r \) (relative) | 9       | 10       | 6.5            | 3               |
| CB effective density of state \( N_c \) (cm⁻³) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) |
| VB effective density of state \( N_v \) (cm⁻³) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) | \(2.2 \times 10^{18}\) |
| Electron Mobility \( \mu_n \) (cm²/Vs)      | 20      | 20       | 2              | \(2 \times 10^4\) |
| Hole Mobility \( \mu_p \) (cm²/Vs)         | 10      | 10       | 2              | \(2 \times 10^4\) |
| Donor density \( N_D \) (cm⁻³)              | \(1 \times 10^{19}\) | \(1 \times 10^{17}\) | 0              | 0               |
| Acceptor density \( N_A \) (cm⁻³)          | 0       | 0        | \(1 \times 10^{15}\)[2] | \(3 \times 10^{18}\) |
| Electron thermal velocity \( v_{thn} \) (cm/s) | \(1 \times 10^7\) | \(1 \times 10^7\) | \(1 \times 10^7\) | \(1 \times 10^7\) |
| Hole thermal velocity \( v_{thp} \) (cm/s)  | \(1 \times 10^7\) | \(1 \times 10^7\) | \(1 \times 10^7\) | \(1 \times 10^7\) |

Table 2. Defect parameters of interface and absorber [14].

| Parameter                               | Defect of absorber | Defect of HTM/Perovskite | Defect of ETM/Perovskite |
|-----------------------------------------|--------------------|--------------------------|--------------------------|
| Defect type                             | Neutral            | Neutral                  | Neutral                  |
| Capture cross section electrons \( \sigma_e \) (cm²) | \(2 \times 10^{15}\) | \(2 \times 10^{15}\) | \(2 \times 10^{16}\) |
| Capture cross-section holes \( \sigma_h \) (cm²) | \(2 \times 10^{15}\) | \(2 \times 10^{15}\) | \(2 \times 10^{16}\) |
| Energetic distribution                   | Gaussian           | Single                   | Single                   |
| Characteristic energy (eV)              | 0.1                | 0.1                      | 0.1                      |
| Energy with respect to reference (eV)   | 0.5                | 0.65                     | 0.65                     |
| Total density (cm⁻²)                    | \((10^{10}-10^{18})\) | \(1 \times 10^{18}\) | \(1 \times 10^{18}\) |

Other parameters such as defect density \( N_t \) in absorption layer is \(2.5 \times 10^{13}\) cm⁻³ using Gaussian distribution and in the other layers are set to \(10^{15}\) cm⁻³. The energy level of the defect is located at the middle of band gap energy with the single distribution in the layers at characteristics energy level 0.1 eV, the type of the defect is neutral, the hole and electron capture cross-section area are \(1 \times 10^{-15}\) cm², and the absorption coefficient for each layer is set to \(10^3\) cm⁻¹. In the simulation, the normal atmospheric conditions are used (AM1.5 G, 300 K) spectrum. The default value is used for the operating point and numerical setting values. The voltage is varied from 0 to 1.3 V. The current-voltage \( J-V \) characteristics of reference cell is shown in Figure 2 and the initial performance parameters are: \( PCE = 12.93\% \), \( FF = 74.99\% \), \( J_{SC} = 21.03\ mA/cm² \), and \( V_{OC} = 0.8202\ V \).

Figure 2. J-V characteristics of the reference cell.
3. Results simulation and Discussions

3.1. Impact of defects in the absorption layer

The performance of perovskite solar cells involved two major procedures which are: one is the generation of a charge carrier, while another is a recombination of charge carrier. In the event of sunlight, the perovskite layer absorbs solar radiation, where the photons are absorbed to produce charged carriers (electrons-holes pair). The electrode sequentially extracts these photo-generated carriers and passes them into the outer in a form of electrical current. Due to poor perovskite layer consistency, a significant number of carriers are lost. In poor perovskite films, a higher value of defect density results in a higher recombination rate, which decreases the propagation length of the carriers and also the lifetime of charge carriers, which can comprehend the fact that there are defects in this layer as a result, it can be decided to investigate recombination as a result of perovskite defects.

3.1.1. Defect density

The impact of defects density in the absorption layer on the performance of the solar cell has been studied by varying the density of the defect from $10^{10}$ cm$^{-3}$ to $10^{18}$ cm$^{-3}$ as shown in Figure 3.

![Figure 3](image)

Figure 3. Performance parameters versus defect density: (a) PCE, (b) FF, (c) $J_{sc}$, (d) $V_{oc}$.

As seen in Figure 3 the power conversion efficiency remains unchanged over the defect density range from $10^{10}$ cm$^{-3}$ to $10^{15}$ cm$^{-3}$. Above the value of $10^{15}$ cm$^{-3}$, the PCE decreased sharply from 12.35% to 0.35%. This can be ascribed to the higher defect density that causes a higher state levels that in turn leads to increasing the trapped region assisted recombination carrier rate. Once a defect density exceeds $10^{16}$ cm$^{-3}$, the $J_{sc}$ reduced rapidly from 21.03 mA cm$^{-2}$ to 2.29 mA cm$^{-2}$ as revealed in figure 2d, which gives an indication to the losses of charge carrier where the trap and recombination processes become significant, while there has been no change in $J_{sc}$ as the density of the defect was below $10^{16}$ cm$^{-3}$. Similar behavior for $V_{oc}$ was observed, it is decreased from 0.82 V to 0.64 V over the defect’s density variation from $10^{15}$ cm$^{-3}$ to $10^{19}$ cm$^{-3}$ with no noticeable change at defect densities below $10^{15}$ cm$^{-3}$. On the other hand, the fill factor (FF) was degraded from 75.02% to 23.99% across the tested defect density range, where the FF remains 75.02% at defect density below $10^{13}$ cm$^{-3}$. It can be deduced from figure 3 that the density of the defect above $10^{15}$ cm$^{-3}$ has a significant impact on the performance
of the PSC device. This interpretation of this phenomenon is due to the fact that because the defect density affects only the active layer which is at the same time the absorber region. It can be observed that as a defect density increases, the lifetime of charge carrier decreases and recombination rate increases, while low defect density results in lesser recombination carrier in perovskite cell.

### 3.1.2. Defects of capture cross-section

The impact of carriers capture cross-section area at absorption layer on the performance of the solar cell has also been investigated, where the capture cross-section was changed from $2 \times 10^{-18}$ cm$^2$ to $2 \times 10^{-10}$ cm$^2$ as shown in figure 4.

![Figure 4](image.png)

**Figure 4.** The effect of capture cross-section on the cell performance: (a) PCE, (b) FF, (c) $J_{sc}$, (d) $V_{oc}$

As seen in figure 4, that all cell performance parameters had almost the same behavior as that of defect density variation. At capture-cross section values below $2 \times 10^{-14}$ cm$^2$, the power conversion efficiency (PCE) is almost constant, whereas, at higher values, the PCE drops rapidly from 12.94% to 0.35%. The fill factor (FF) is strongly influenced by increasing the capture cross-section area, where FF decreased slightly below $2 \times 10^{-13}$ cm$^2$, however, it was reduced sharply from 72.48% to 23.99% for higher capture cross-section area. The $J_{sc}$ degradation from 21.03 mA·cm$^{-2}$ to 2.29 mA·cm$^{-2}$ is noticed when the capture cross-section was varied from $2 \times 10^{-14}$ cm$^2$ to $2 \times 10^{-10}$ cm$^2$. Also, it was observed that when the capture cross-section area was increased the $V_{oc}$ reduced slightly from 0.82 V to 0.64 V. The PCE reduces from the maximum value from efficiency about 12.59% and FF decrease from 75.02% below 51.1% and $J_{sc}$ around 18.74% $V_{oc}$ about 0.18%. The results in the figure 4 showed that the impact of the capture cross-section exhibited similar behavior to the influence of defects density in the absorption layer. This behavior can be interpreted as the lifetime of carriers is determined by the trap density and carriers capture cross-section, thus when the capture cross-section increase, the carrier lifetime decrease due to dimension of defect trap increase leads to significantly reduced solar cells performance.

### 3.2. Impact of defects in the interface layer

Two interfaces (ETM/absorber) and (absorber/HTM) were presented in the proposed structure of the cell and the impact of defects in ETM/absorber interface layer on the performance of the cell was investigated. The defect parameters of the two interface layers are shown in table 2. The influence of
the defect density at ETM/absorber interface layer on the solar cell parameters has been changed from $10^{11}\text{cm}^{-2}$ to $10^{20}\text{cm}^{-2}$ while the other variables were kept unchanged. The results are shown in figure 5.

![Figure 5. Change in cell parameters (a) PCE, (b) FF, (c) $J_{sc}$, (d) $V_{oc}$ in relation to the defect density on the ETM/absorber interface layer.](image)

It is seen in figure 5 that the increase in the defect density results in a slight decrease in the $PCE$, $FF$, and $J_{sc}$, while the $V_{oc}$ has shown no significant change. It can also be noticed that the cell parameters exhibited a small change for defect densities greater than $10^{14}\text{cm}^{-2}$ below the defect density of $10^{14}\text{cm}^{-2}$, the $PCE$ reduced from maximum efficiency by about 1.35% and $FF$ decreased from 78.10 by around 3%, and $J_{sc}$ decrement was less than 1.14% while $V_{oc}$ remained unchanged. The solar cell performance was trivially influenced by the density of the defect at the ETM interface. In HTM/absorber interface layer, it is observed no prominent impact of the defect density on the performance parameters in PSC. Due to the interfaces are represented as defects when the defect density was varied over the tested range, the cell performance suffered a slight reduction.

4. Conclusion

In the present work, the effect of defect density and carriers capture cross section area at the absorber layer and defect density at the ETM/Perovskite interface layer in perovskite solar cells with planar structure FTO/TiO$_2$/CH$_3$NH$_3$PbI$_3$/Spiro-OMeTAD were studied by one dimensional Solar Cells Capacitance Simulator (SCAPS-1D). The results showed that when the defect density increased in the absorption layer, the $PCE$, $FF$, and $J_{sc}$ are dropped sharply, however, $V_{oc}$ was slightly decreased. Furthermore, it was noticed that a higher capture cross-section area causes significant degradation in the cell performance and has shown similar behavior of the defect density effect. The cell parameters such as $PCE$, $FF$, and $J_{sc}$ decreased slightly when the defect density at ETM/absorber interface layer was changed from $10^{11}\text{cm}^{-2}$ to $10^{20}\text{cm}^{-2}$ and showed that the $V_{oc}$ has no significant impact. It was also shown that the influence of defect density in the interface layer was trivial when compared with the absorption layer. Further investigation is needed to explore the effect of high defect densities in other materials rather than Spiro-OMeTAD such as Cu$_2$O and CuI.
5. References

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