Efficiency of TiO₂/Perovskites/Cu₂O Solar Cells with Optimal Thickness at Varying of Environment Temperature

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Abstract

Perovskite solar cells become another field for conventional solar cells achieving an output of 22.1 percent in eight years (2008-2016) short period. There is reason to believe that PSCs are a strong competitor in the photovoltaic field with silicone and CIGS solar cells. The well understanding of the operation mechanism of PSCs is essential and mandatory to furtherly improve device performance. The shape and excitation type is like to inorganic semiconductor solar cells. This work is concerned about the design and studies of lead-based perovskite solar cell model with the flexible architecture of ITO/TiO₂/CH₃NH₃PbI₃/Cu₂O/Au and analyzed using the solar cell capacitance simulator (SCAPS-1D), we study the effects of the thicknesses for all active materials which are ETM, HTM and Perovskites in addition to environment temperature on the main parameters of our device solar cells.

Method/Analysis:

Solar cell device assessment is conducted using a Solar Cell Power Simulator(SCAPS). This is a computer-based software tool and is well equipped to conduct research into photovoltaic structures with barriers to homo and heterojunctions, multi-junctions, and Schottky. This model optimizes various parameters such as the thickness, Electron Transport Material (ETM) (ND and NA) doping concentrations, and Hole Transport Material (HTM). Achievement and simulates electrons and holes based on the Poisson's and continuity equation. The effected thickness of CH₃NH₃PbI₃ different from 0.2μm to 1μm and the finest results are observed at 0.2μm.

Improvements: Efficiency is constant at different temperatures when using the finest thickness for the material where the efficiency reached 21%.

Introduction

Lead-based solar cells (PSCs) based on methylammonium halide perovskite have attracted considerable interest in materials research, chemistry, and physics. The halide perovskite with the chemical formula of A₈X₃ (A is organic and normally methyl ammonium (CH₃-NH₃ + ); B is commonly plumbum, and X is halogen) as solar cells absorbers was firstly published at 2009 [1]. Korean researchers (Yang, Noh, and...
coworker) recently announced that the maximum verified record of conversion efficiency is 20.1 percent [2]. Despite the rapid increase in efficiency from 3.8% to 20.1% after several years of intensive work into manufacturing innovation and performance promotion, the efficiency of ssPSCs still lags behind the Shockley-Queisser theoretical maximum value (31.4%) [3]. Following the first study of the content of solar cells in 2009 [4], perovskite solar cells (PSCs)’s Power Conversion Efficiencies (PCEs) have now reached a certified value above 23 percent [5]. PSCs have achieved comparable photovoltaic efficiency to copper indium gallium selenide (CIGS) solar cells (22.9%) and approach monocristalline silicon solar cells (26.1%) for single-joint silicon cells without concentrators [5]. The related simulation work has given the basic information from the literature to build this model [6–10]. In this device, we examined and analyzed the effect of absorber layer properties (thickness) and the impact of HTM and ETM doping on system output SCAPS is software for window application, Developed with laboratory windows / CVI of a national instrument at the University of Ghent. The software is arranged in a Set of panels where the consumer can set parameters or calculate outcomes [11]. SCAPS analyzes model physics and explains the recombination profiles, the distribution of electric fields, the carrier transport mechanism, and the individual current densities. Generally, ETL and HTL are used in the PSCs for broad bandgap hole blocking and electron blocking materials respectively. The PSCs use different types of organic and inorganic materials, such as TiO$_2$, ZnO, SnO$_2$, and Al$_2$O$_3$, as ETL [12,13]. TiO$_2$ among them is the most promising material for the ETL because of its wide bandgap, high stability, and attractive bending with perovskite material [14]. Specific TiO$_2$ nanostructures such as nanotube, nanosheets, nanoparticles, nanorods, and nanowires were used in highly effective PSCs as an ETL [15–18]. It is stated that the weight, diameter, and morphology of the TiO$_2$ nanostructures influence PSC performance [19]. However, due to its amazing transport and robustness with perovskite materials, TiO$_2$ is preferred over other nanostructures within the PSCs[20]. By integrating Cu$_2$O as a material of p-type with a narrow bandgap (1.9–2.0eV) [21] The solar absorption, beneficial bandgap, and good rectification properties could be enhanced; inevitable in contributing to high thin-film efficiency.

**Numerical modeling and Device simulation**

There are several modeling and simulation tools available today. Software for solar cells in which the Analysis program for solar cells is in one dimension is software SCAPS. Various types of semiconductor materials were used for many solar cell modules. For the work currently underway, SCAPS used to model the TiO$_2$/CH$_3$NH$_3$PbI$_3$/Cu$_2$O perovskite solar cells in perovskite. The nanostructure of TiO$_2$/CH$_3$NH$_3$PbI$_3$/Cu$_2$O solar hetrojunction cells was simulated at different working point Thickness and was subjected to different ambient temperatures for heat investigation using SCAPS.

**Solar cells capacitance simulation (SCAPS)**
The simulation package of solar cell structures, first adapted at Gent University using the CdTe and CuInSe$_2$ family structure [22]. The SCAPS explains the output of a solar cell mathematically using finite differential methods in solar cell physics to solve Differential equations with laws and reference number. SCAPS is a numerical solution of the two poison and continuity equations on boundary conditions suited to one or two dimensions [23]. The express of equations as shown below:

\[
\nabla^2 V = -q / \varepsilon (p - n + N_D - N_A) \quad \text{(1)}
\]

\[
\nabla J_p = q (G - R) \quad \text{(2)}
\]

\[
\nabla J_n = q (R - G) \quad \text{(3)}
\]

\[
J_p = -q \mu_p PV_p - KT \mu_p V_p \quad \text{(4)}
\]

\[
J_n = -q \mu_n PV_n + KT \mu_n V_n \quad \text{(5)}
\]

\[
V_p = V - (1 - \gamma) \Delta G / g \quad \text{(6)}
\]

\[
V_n = V + \gamma \Delta G / g \quad \text{(7)}
\]

Equations 5 and 6 reflect the current density of the hole and the electron. Where $V_b$ and $V_n$ are the potential effectives expressed in Eqs 6 and 7. $\Delta G$ is band structure variance, $\mu_n, \mu_p$ reflects electron and hole mobility respectively. A typical CH$_3$NH$_3$PbI$_3$ based solar cell structure consists of an absorber layer and at the top p-type (Cu$_2$O) and n-type (TiO$_2$) is arranged at the bottom side. The cell is illuminated schematically as shown in Figure 1.

![Figure 1](image)

**Figure 1.** Schematic representation device architecture (ITO/TiO$_2$/CH$_3$NH$_3$PbI$_3$/Cu$_2$O/AU).

SCAPS solves the Basic semiconductor equations in 1-Dimension under steady-state condition.
**Figure 2:** Explains the simulation process using SCAPS.

**Simulation results**

**SCAPS simulation of Cu$_2$O/Perovskite/ TiO$_2$**

Note that all simulation parameters for each layer in the device are carefully selected from those reported experimental data and other literature [24]. Table 1 summarizes all of the primary parameters for simulation use.

**Table 1:** Material properties of ETM, absorber, and HTMs.

| Parameters                              | Cu$_2$O | CH$_3$NH$_3$PbI$_3$ | TiO$_2$ |
|----------------------------------------|---------|---------------------|---------|
| Band gap (eV)                          | 2.17    | 1.5                 | 3.26    |
| Electron affinity (eV)                 | 3.20    | 3.9                 | 4.2     |
| Dielectric permittivity                | 7.11    | 10                  | 10      |
| CB effective density of states (1/cm$^2$) | 2.02E+17 | 2.75E+18           | 2.0E+17 |
| VB effective density of states (1/cm$^2$) | 1.10E+19 | 3.9E+18             | 6.0E+17 |
| Electron mobility (cm$^2$/v.s)         | 2.000E+2| 1.00E+1             | 100     |
| Hole mobility (cm$^2$/v.s)             | 8.00E+18| 1.0E+1              | 25      |

A schematic representation of the structure solar cells which simulated by SCAPs is shown in Figure 3
Figure 3: SCAPS panel showing the Cu$_2$O/CH$_3$NH$_3$PbI$_3$/TiO$_2$ heterojunction solar cells definition.

The efficiency is calculated from equation (8)

$$\eta = FF \times \frac{(V_{oc} \times J_{sc})}{P_{in}}$$

Figure 4: Device structure and energy level diagram of the TiO$_2$/CH$_3$NH$_3$PbI$_3$/Cu$_2$O/Au.
Table 2: Devise Parameters use in the numerical analysis.

| Right contact electrical properties (Au)         |                   |
|-----------------------------------------------|-------------------|
| Thermionic emission / surface recombination   | $10^6$            |
| Velocity of electron (cm/s)                   |                   |
| Thermionic emission / surface recombination   | $10^7$            |
| Velocity of hole (cm/s)                       |                   |
| Metal (Au) work function (ev)                 | 5.1               |

| Left contact electrical properties             |                   |
|-----------------------------------------------|-------------------|
| Thermionic emission / surface recombination   | $10^7$            |
| Velocity of electron (cm/s)                   |                   |
| Thermionic emission / surface recombination   | $10^6$            |
| Velocity of hole (cm/s)                       |                   |
| work function of ITO (ev)                     | 4.4               |

Result and Discussion

1. Effect of the Cu$_2$O layer thickness change on solar cells

The absorber layer should be set for optimum thickness to absorb the maximum number of photons and to generate electron-hole pairs. Absorber layer thickness has been ranged from 1 $\mu$m to 5 $\mu$m. As the thickness of the absorber layer increases the longer wavelength of the illumination induces a fair amount of electron-hole pair generation. By rising the absorber layer thickness the depletion layer gets very close to the back contact and more electrons are captured for recombination by the back contact. By these fewer electrons will participate in the generation process, and finally, leads to the reduced fill factor and increase efficiency. Figure 5 represents the variation of PV parameters with the thickness of the absorber layer. The graph shows an efficiency gain as we turn from the thinner absorber to the thicker absorbers due to the increased exciton output. But there is a quick drop in the fill factor.

The reason behind that is fill factor is strongly affected by the electric field and the electric field in the absorber decreases with increasing the forward bias. It will lead to a reduced collection of carriers, which was assisted by the electric field. The higher fill factor needs a quality absorber. By observing the Voc/thickness graph, we can say that there is increases Voc by increasing the thickness. From Jsc/thickness graph; short circuit current increases, by increasing the thickness. This is because the increase of spectral response at the longer wavelengths by increasing the thickness So it can get the best efficiency and fill factor at a thickness of 2 $\mu$m where the efficiency reaches 3.4 and full factor is 58.9. Table number three shows the drawing data.

Table 3: Variation of Thickness for Cu$_2$O with device parameters.
Table 4

| Thickness (μm) | \( V_{oc} \) (V) | \( J_{sc} \) (mA/cm²) | F.F (%) | \( \eta \) (%) |
|---------------|------------------|------------------------|---------|---------------|
| 1             | 0.884            | 5.598                  | 58.20   | 2.88          |
| 2             | 0.934            | 5.612                  | 58.9    | 3.4           |
| 3             | 0.974            | 5.620                  | 57.24   | 3.13          |
| 4             | 1.011            | 5.625                  | 56.22   | 3.20          |
| 5             | 1.039            | 5.629                  | 55.49   | 3.25          |

Figure 5. Variation of PV parameters by varying the thickness of Cu₂O.

2. Effect of the TiO₂ layer thickness change on solar cells

The thickness of the absorber layer has been varied from 0.2 μm to 1.2 μm. Figure 6 represents the variation of PV parameters with the thickness of the absorber layer. The graph represents that the efficiency, \( V_{oc} \), and \( J_{sc} \) are decreased as we go from the thinner absorber to the thicker absorbers. But there is an increased fill factor. Table number four shows the drawing data. So it can figure out that the best PV parameter at 0.2 μm which are listed in Table 4.
Table 4: Variation of Thickness for TiO₂ with device parameters.

| Thickness (μm) | V<sub>oc</sub> (V) | J<sub>sc</sub> (mA/cm²) | F.F (%) | η (%) |
|---------------|-------------------|----------------------|--------|------|
| 0.2           | 0.8849            | 5.5980               | 58.20  | 2.88 |
| 0.3           | 0.8845            | 5.5133               | 58.23  | 2.84 |
| 0.4           | 0.8842            | 5.4599               | 58.25  | 2.81 |
| 0.5           | 0.8840            | 5.4176               | 58.27  | 2.79 |
| 0.6           | 0.8838            | 5.3809               | 58.28  | 2.77 |
| 0.7           | 0.8836            | 5.3481               | 58.30  | 2.75 |
| 0.8           | 0.8835            | 5.3183               | 58.31  | 2.74 |
| 0.9           | 0.8833            | 5.2908               | 58.32  | 2.73 |
| 1             | 0.8832            | 5.2655               | 58.33  | 2.71 |
| 1.1           | 0.8831            | 5.2419               | 58.33  | 2.70 |
| 1.2           | 0.8830            | 5.2198               | 58.34  | 2.69 |

Figure 6: Variation of PV parameters by varying the thickness of TiO₂.

3. Effect of the CH₃NH₃Pbl₃ layer thickness change on solar cells

The thickness of the absorber layer has been varied from 0.2μm to 1μm. Figure 7 represents the variation of PV parameters with the thickness of the absorber layer. The graph represents that the efficiency, Voc, and Jsc are decreased as we go from the thinner absorber to the thicker absorbers. But there is an increased fill factor. Table number five shows the drawing data. One shows that the optimal thickness for
perovskits solar cells is 0.2 micrometer as listed in table 5 where 0.2-micrometer thickness corresponds to the efficiency of 9.12.

**Table 5:** Variation of Thickness for CH$_3$NH$_3$Pbl$_3$ with device parameters.

| Thickness (μm) | V$_{oc}$ (V) | J$_{sc}$ (mA/cm$^2$) | F.F (%) | η (%) |
|---------------|-------------|---------------------|--------|-------|
| CH$_3$NH$_3$Pbl$_3$ |             |                     |        |       |
| 0.2           | 1.1739      | 40.105              | 19.37  | 9.12  |
| 0.3           | 1.1325      | 22.391              | 19.30  | 4.89  |
| 0.4           | 1.0594      | 12.640              | 27.05  | 3.62  |
| 0.5           | 1.043       | 8.271               | 38.51  | 3.32  |
| 0.6           | 1.0403      | 6.411               | 48.90  | 3.26  |
| 0.7           | 1.0397      | 5.803               | 53.87  | 3.25  |
| 0.8           | 1.0395      | 5.660               | 55.19  | 3.25  |
| 0.9           | 1.0394      | 5.634               | 55.44  | 3.25  |
| 1             | 1.0394      | 5.629               | 55.49  | 3.25  |

**Figure 7:** Variation of PV parameters by varying the thickness of CH$_3$NH$_3$Pbl$_3$.

4. Effect of annealing temperatures for CH$_3$NH$_3$Pbl$_3$

The results of simulation I-V characteristic such as PCE, FF, J$_{sc}$, and V$_{oc}$ of the perovskite solar cells with varying environment temperature as shown in Table 6 where the highest efficiency is 9.12% with J$_{sc}$ = 40.105 mA/cm$^2$, FF = 19.37% and V$_{oc}$ = 1.1739
is achieved when the temperature at 238 K, therefore the best result at very low temperature to be very appropriate to work in space. When the temperature is increasing from 283 K to 333 K, the PCE, and Jsc degrees due to reducing in the generation of the electron-hole pairs in the perovskite materials with increasing temperature as shown in Figure 8. From Figure 8 the open-circuit voltage digresses gradually with increasing temperature, it can adjust the efficiency with temperature due to control of the recombination, generation, and a collection of the charge carriers so the best temperature of perovskit solar cells with CH₃NH₃PbI₃ as PVSC is 283 k. In the same time, it can be seen that the device of perovskite solar cells of CH₃NH₃PbI₃ has very high stability with temperature as shown in the Figure 8 the changing is small in parameter, which can conclude that the stability base temperature is very stable and resistant to temperature, is it can use in high temperature country.

| T(K) | V_{oc} | J_{sc} | FF | Efficiency % |
|------|--------|--------|----|--------------|
| 283  | 1.1739 | 40.105 | 19.37 | 9.12          |
| 293  | 1.1325 | 22.391 | 19.30 | 4.89          |
| 303  | 1.0594 | 12.640 | 27.05 | 3.62          |
| 313  | 1.043  | 8.2718 | 38.51 | 3.32          |
| 323  | 1.0403 | 6.4117 | 48.90 | 3.26          |
| 333  | 1.0397 | 5.8030 | 53.87 | 3.25          |

Table 6: The parameter of the Cu₂O/ CH₃NH₃PbI₃/TiO₂ heterojunction solar cell.

![Figure 8: The variation of solar cell parameters with the temperature.](image)

5. Effect of different back contact material
Simulation has been done using gold (Au), aluminum (Al), tin (Sn), silver (Ag), iron(Fe), carbon (C), cobalt (Co), nickel (Ni), platinum (Pt) and cooper (Cu) as back contact for inverted PSC. Figure 9 illustrated a simulated check of the efficiency of different back contact materials. The efficiency of solar cells increases with increasing as a function of metal work function. Improves performance with increased metal work function value due to the major carrier barrier height increase thus efficiency increase. Table 6 shows effect of various metal contact on the efficiency of the cell. Pt is the most suitable back contact in inverted PSC.

Table 6: Shows effect of various metal contact on efficiency of the cell.

| Work function (ev) | V_{oc}  | J_{sc}  | FF   | Efficiency% |
|--------------------|---------|---------|------|-------------|
| 4.2                | 0.2536  | 1.0420  | 23.96| 0.06        |
| 4.3                | 0.3530  | 3.1106  | 10.64| 0.12        |
| 4.4                | 0.3530  | 3.1106  | 10.64| 0.12        |
| 4.5                | 0.5525  | 13.222  | 12.88| 0.94        |
| 4.6                | 0.6525  | 17.1827 | 16.12| 1.81        |
| 4.7                | 0.7527  | 21.6964 | 17.34| 2.83        |
| 4.8                | 0.8525  | 26.7033 | 17.52| 3.99        |
| 4.9                | 0.9525  | 31.8441 | 17.52| 5.31        |
| 5                  | 1.0666  | 36.4154 | 17.69| 6.87        |
| 5.1                | 1.1650  | 39.4918 | 18.66| 8.58        |
| 5.12               | 1.1711  | 39.8264 | 19   | 8.86        |
| 5.15               | 1.1714  | 40.138  | 19.42| 9.15        |
| 5.25               | 1.1745  | 40.3808 | 19.81| 9.40        |
| 5.65               | 1.3248  | 43.0058 | 30.21| 16.67       |

Figure 8: The variation of work function with efficiency.
Conclusions

In short, we have simulated the perovskite solar cells using two types of HTM for Cu$_2$O and ETM for TiO$_2$ and Perovskit CH$_3$NH$_3$PbI$_3$. In this study, optimization was an investigation for Cu$_2$O, TiO$_2$ and CH$_3$NH$_3$PbI$_3$, the observation for each semiconductor materials and after that also the study with a variety of temperature where the best efficiency reach to 9.12% at 283 K to be amazing device work at low temperature, especially in space, in the same time it has high stability with a variety of environment of temperature. Also in this research, we dealt with the change of the work function with efficiency to optimize the work function, and show the height level efficiency corresponding to 5.65 ev work function, the efficiency much improve to reach 16.67%.

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