Perovskite solar cells based on CH$_3$NH$_3$SnI$_3$ Structure

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Abstract: In recent years, organic-inorganic perovskite solar cells have attracted considerable interest in the photovoltaic research community because of its ease of processing, low production costs, super light-harvesting characteristics, and relatively high performance, making it more desirable than other current solar cell materials. Lead-based perovskites (CH$_3$NH$_3$PbX$_3$, X=Cl, I, Br) solar cells have recently achieved high efficiency of ~19.3 percent, well exceeding most thin-film and organic solar cells' efficiencies. The presence of lead, toxic material in these solar cells, therefore poses serious challenges to our health and the environment. ‘Tin’ is nontoxic and stands as a replacement to ‘lead’ for commercial purposes. In halide based Perovskites possess a potential for higher quantum efficiency because of their enhanced light absorption capability due to the wide-ranging absorption spectrum in the visible region with a comparatively lower band gap of 1.3 eV than lead-based Perovskites. In this work, we have modeled a tin-based perovskite simulation model with FTO Glass / ZnO / CH$_3$NH$_3$SnI$_3$ / Cu$_2$O / Pt. novel architecture and analyzed using the SCAPS-1D, which is well suited for studying photovoltaic architecture. Use this software method and we analyzed the thickness, fault density, and operating temperature of the model by simulating under various conditions. With the optimize the thickness to be (0.03 µm) corresponding best efficiency among another thickness of perovskites, and other layers, the defect density of absorber layer (10$^{17}$ cm$^{-3}$ ) the encouraging result of maximum power conversion efficiency(PCE) reached to 9.27%, the short-circuit current density(Jsc) is 46.569 mA/cm$^2$, and fill factor(FF) is 31.17% and open-circuit voltage(Voc) is 0.637 V is calculated.

1-Introduction

Due to simple processing techniques and low production costs compared to traditional silicon-based solar cells and high PCE, organometal halide perovskite solar cells (PSCs) in the field of optoelectronic devices have gained much interest from the research community in recent years [1]. Since the first introduction of CH$_3$NH$_3$PbX$_3$ PSCs, efficiency has grown exceptionally, from 3.8% in 2009 to 25.2% in 2019 [2]. While PSC based on lead has high efficiency because it contains lead, it is toxic and can cause health and ecological hazards[3]. The toxicity of traditional perovskite solar cells can be avoided by using CH$_3$NH$_3$SnI$_3$, which has a direct 1.30 eV bandage as an absorber layer. This has the most acceptable optical properties and the light-absorption spectrum of all CH$_3$NH$_3$BX$_3$ optoelectric compounds (B = Sn, Pb; X = Cl, Br, I)[4]. However, recent studies have shown that ZnO can be used as a proper substitute for TiO2 as the ETM layer without affecting PSC performance significantly.
[5, 6]. It has a 3.37 eV, a clear band gap. This wide-band gap contributes to high mobility in the transport of electrons. Such a solar cell’s performance can be further improved by using the nanostructured ETM thin film. To observe their influence on efficiency, inorganic materials semiconductors were used for an HTM layer, we considered in the organic semiconductor of the Cu$_2$O HTM layer. From I-V characteristics of all three structures, it was evident that the highest efficiency can be namely, Poisson’s (1) and continuity equations for holes (2) and electrons (3) as follows:

\[
\frac{d}{dx}(-\varepsilon(x) \frac{d\psi}{dx}) = q \left[ p(x) - n(x) + N_a^+ (x) - N_a^- + p_t (x) - n_t (x) \right] ......(1)
\]

\[
\frac{dp_n}{dt} = G_p - \frac{p_n - p_n0}{\tau_p} - p_n \mu_p \frac{d\eta}{dx} - \mu_p \eta \frac{dp_n}{dx} + D_p \frac{d^2 p_n}{dx^2} .......(2)
\]

\[
\frac{dn_p}{dt} = G_n - \frac{n_p - n_p0}{\tau_n} + n_p \mu_n \frac{d\eta}{dx} + \mu_n \eta \frac{dn_p}{dx} + D_n \frac{d^2 n_p}{dx^2} .......(3)
\]

Here \(\varepsilon\) is dielectric constant, \(W\) is electrostatic potentiality, \(q\) is the electron charge, \(D\) is diffusion coefficient, \(n\) is permittivity and \(n, p, n_t, p_t\) are free electrons, free holes, trapped electrons, and trapped holes respectively. \(N_a^-\) refers to the concentration of ionized acceptor-like doping and \(N_d^+\) for ionized donors such as doping [7].

1.1. Perovskites structure

Perovskite generally refers to any crystalline material with chemical formula \(ABX_3\) [8] as shown in Figure 1.

![Perovskite crystal structure](image)

Figure 1. A typical crystal structure of a Perovskite [9].

Most of the materials in perovskite solar cells served as a photo-active layer consist of an organo-metal halide. Organic-cation (A) usually involves (methyl-ammonium ‘MA’ and formamide ‘FA’) with several divalent metal cations (B) such as Cu$_2^+$, Fe$_2^+$, Mn$_2^+$, Pb$_2^+$, Sn$_2^+$, etc.. These cations were mixed with a halide (X), such as F$^-$, Cl$^-$, Br$^-$, and I$^-$ anions. The mixture of the various ratios of A-cation, B-cation, and X-anion can be obtained from specific perovskite materials[10]. Direct cation or anion replacement may result in distorted perovskite or non-perovskite structure. Goldschmidt Tolerance Factor (GTF) is a
dimensionless empirical index that can predict the regular crystal structure of a perovskite [11].

1.2. Numerical Simulations

Simulation is a critical technique for realizing a deep insight into the physical activity, the feasibility of the physical explanation suggested, and the impact of physical changes on the efficiency of the solar cell devices. There are several simulation models for solar cell simulation (SCAPS, AMPS, SCAP, etc.). SCAPS (Solar Cell Power Simulator) is a one-dimensional simulation software with seven input layers of semiconductors developed by a group of solar cell researchers from the Department of Electronics and Information System, University of Ghent, Belgium [12]. Thus SCAPS like 1D simulator can be employed to simulate the perovskite-based solar cells

![Simulation Diagram]

1.3. SCAPS simulation of CuO/Perovskite/ZnO

Note that all simulation parameters for each layer in the architecture are carefully selected from those reported experimental data and other literature [13]. Table 1 summarizes all the primary parameters used in the simulation.

Table1: The proposed design input parameters for its different layers [14-19]

| Parameters                      | Cu₂O       | CH₃NH₃SnI₃ | ZnO       |
|--------------------------------|------------|------------|-----------|
| Band gap (eV)                  | 2.17       | 1.3        | 3.3       |
| Electron affinity (eV)         | 3.20       | 4.17       | 4.0       |
| Dielectric permittivity        | 7.11       | 8.2        | 9.0       |
| CB effective density of states (1/cm²) | 2.02E+17  | 1e+18      | 3.7 x 10¹⁴ |
| VB effective density of states (1/cm²) | 1.10E+19  | 1e+18      | 1.8 x 10¹⁹ |
| Electron mobility (cm²/V.s)    | 2.000E+2   | 1.6        | 100       |
| Hole mobility (cm²/V.s)        | 8.00E+18   | 1.6        | 25        |
Table 3: Devise Parameters use in the numerical analysis

| left contact electrical properties (Pt.) | right contact electrical properties |
|----------------------------------------|-------------------------------------|
| Thermionic emission /surface recombination Velocity of electron (cm/s) | 10^5 |
| Thermionic emission /surface recombination Velocity of hole (cm/s) | 10^7 |
| Metal (Pt.) work function (ev) | 5.65 |
| Thermionic emission /surface recombination Velocity of electron (cm/s) | 10^5 |
| Thermionic emission /surface recombination Velocity of hole (cm/s) | 10^7 |
| the work function of ITO (ev) | 4.4 |

Result and discussion

1-Effect of a thickness of Cu2O 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 1μm to 5μm. 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. Figure 2 represents the variation of PV parameters with the thickness of the absorber layer The graph shows an efficiency, filling factor, voltage open circuit, and current density increases with increasing thickness. So it can get the best efficiency at a thickness of 4.5 μm where the efficiency reaches (4.69). Table number three shows the drawing data.

Table 3 Variation of Thickness for Cu2O with device parameters.

| Thickness (μm) | Voc (volt) | Jsc (mA/cm²) | FF | Efficiency % |
|----------------|------------|--------------|----|--------------|
| 0.5            | 0.9707     | 31.707       | 13.34 | 4.31        |
| 1.5            | 0.974      | 33.764       | 13.45 | 4.42        |
| 2.5            | 0.9757     | 34.399       | 13.52 | 4.54        |
| 3.5            | 0.976      | 34.792       | 13.60 | 4.62        |
| 4.5            | 0.9777     | 35.087       | 13.68 | 4.69        |
2. Effect of thickness of the CH3NH3SnI3 on the solar cell.

Absorber layer thickness has a big influence on the solar cell's overall performance. CH3NH3SnI3 has ranged in thickness from 0.03 μm to 0.07 μm. Fig. 3 reflects the variation of the photovoltaic parameters with perovskite layer thickness. When the thickness of the perovskite layer increases, the efficiency of the solar cell decreases, which is considered to be the optimum thickness for the solar cell at 0.03 μm, the efficiency value is (8.24). The results decrease in the short circuit current (Jsc) with an increase in thickness. While effectiveness decreases after a certain thickness size. Causes Voc insensorial and ff decorative. Figs. 3 Shows the outcome of the simulation. The Voc increase due to degrees the current as a result of the nature of perovskites which has very high density, therefore, its make difficulty to excess the electrons, and increase resistivity, therefore, it cause accumulation electrons in one side of perovskite, it can see the increase of the Voc, and reduce, Jsc, and FF with increase the thickness.
Table 4 Variation of Thickness for CH$_3$NH$_3$SnI$_3$ with device parameters

| Thickness (µm) | Voc (volt) | Jsc (mA/cm$^2$) | FF | Efficiency % |
|---------------|------------|-----------------|----|--------------|
| 0.03          | 0.689      | 46.502          | 25.70 | 8.24         |
| 0.04          | 0.719      | 45.823          | 23.21 | 7.66         |
| 0.05          | 0.750      | 45.105          | 21.13 | 7.15         |
| 0.06          | 0.780      | 44.295          | 19.41 | 6.71         |
| 0.07          | 0.810      | 43.416          | 17.98 | 6.33         |

3. Effect of thickness of the ZnO on the solar cell.

The absorber layer should be set for optimum thickness to absorb the maximum number of photons and to produce electron-hole pairs. Absorber layer thickness has been varied from 0.05µm to 0.250 µm. When the thickness of the absorber layer increases the longer wavelength of the illumination produces a good amount of electron-hole pair generation. Figure 4 indicates variation in the thickness of an absorber sheet of PV parameters. By looking at the Voc / thickness graph we can say that by increasing its thickness, increase the voc till the thickness 0.15 where Voc reached to 0.7 then declined and reduced gradually due it got best accumulation charge across the device of solar cells, while the highest value of Jsc at 0.05 where the Jsc reached to 45 then the Jsc degrees gradually with increase the thickness due to increase the resistivity with thickness. From Jsc/ thickness graph; the short circuit current decrease, by increasing the thickness. From the efficiency/thickness graph we can say
that there is decreasing with increasing thickness and filling factor increases with an increasing thickness which is related to increase the Voc. we can observe that from the graph. optimum thickness at (0.05) the efficiency is (8.24). Table 5 shows the drawing data.

Table 5 Variation of Thickness for ZnO with device parameters

| Thickness (µm) | Voc (volt) | Jsc (mA/cm²) | FF  | Efficiency % |
|---------------|-----------|--------------|-----|--------------|
| 0.05          | 0.689     | 46.502       | 25.70 | 8.24         |
| 0.100         | 0.748     | 43.986       | 18.83 | 6.20         |
| 0.150         | 0.780     | 38.964       | 17.06 | 5.19         |
| 0.200         | 0.754     | 33.534       | 18.64 | 4.72         |
| 0.250         | 0.734     | 29.038       | 21.03 | 4.48         |

Figure 4. Variation of PV parameters by varying the thickness of ZnO.

4- Effect of the defect state of the interface defect layers Cu₂O/CH3NH3SnI3/ZnO

Generation, recombination, transport cycle occurs within the absorber layer, so the consistency of the absorber layer and the parameters of the defects significantly affect the output of the device[20]. The variation of parameters for solar cells, with the defect density, is as shown in Fig-4. The defect density is varied in the simulation model from 1 * 10¹⁷ cm⁻³ to 6 * 10¹⁷ cm⁻³ It has been observed that, if the absorber layer of defect density increases from 1 * 10¹⁷ cm⁻³ to 6 * 10¹⁷ cm⁻³, the performance, filling factor and current density of the photovoltaic parameters decrease with increasing defect but voltage increases. An abrupt reduction in PV parameters with an increase in defect density indicating that the increased defects act as a recombination center that decreases carrier lifetime. The optimal density of defects at 1 * 10¹⁷ = 9.27%, off=31.17, Jsc=46.569 and Voc=0.637.
Table 6 Defect for CH$_3$NH$_3$SnI$_3$ with device parameters

| Defects Nt(1/cm$^3$) | Voc (volt) | Jsc (mA/cm$^2$) | FF  | Efficiency % |
|----------------------|------------|----------------|-----|--------------|
| 1*10$^{17}$         | 0.637      | 46.569         | 31.17 | 9.27        |
| 2*10$^{17}$         | 0.663      | 46.563         | 28.05 | 8.66        |
| 3*10$^{17}$         | 0.677      | 46.520         | 26.81 | 8.44        |
| 4*10$^{17}$         | 0.693      | 46.497         | 25.83 | 8.33        |
| 5*10$^{17}$         | 0.689      | 46.483         | 25.79 | 8.27        |
| 6*10$^{17}$         | 0.708      | 46.472         | 24.99 | 8.22        |

Figure 5: Defect density of the Cu$_2$O/CH$_3$NH$_3$SnI$_3$/ZnO solar cells

5- Influence of operating temperature

Working temperature plays a major role in the performance of a device. Generally, the testing temperature of a solar cell device is at 333.15 K, but at the installed conditions, the working temperature is more than 333.15 K. In this simulation model Pt/Cu$_2$O/CH$_3$NH$_3$SnI$_3$/ZnO/ITO the operating temperature varied from 333.15K to 233.15 K, then the changes in the characteristics are observed and given in Fig6. As the temperature decreases from 333.15 K to 233.15 K, then the efficiency drops to 8.22% and fill factor is 24.99%, Jsc=46.472 mA/cm$^2$, Voc=0.708V at 233.15K, optimum efficiency=9.27, Jsc=46.569 mA/cm$^2$, ff=31.17 and Voc=0.637 at temperature 333.15 K the efficiency, filling factor, current density decreases with decreasing temperature while Voc increasing.
Table 7. The parameter of the Cu$_2$O/CH$_3$NH$_3$SnI$_3$/ZnO heterojunction solar cells

| Temperature (K) | Voc (Volt) | Jsc (mA/cm$^2$) | FF | Efficiency % |
|----------------|------------|-----------------|----|--------------|
| 333.15         | 0.637      | 46.569          | 31.17 | 9.27     |
| 313.15         | 0.663      | 46.563          | 28.05 | 8.66     |
| 293.15         | 0.677      | 46.520          | 26.81 | 8.44     |
| 273.15         | 0.693      | 46.497          | 25.83 | 8.33     |
| 253.15         | 0.689      | 46.483          | 25.79 | 8.27     |
| 233.15         | 0.708      | 46.472          | 24.99 | 8.22     |

Figure 6: The variation of solar cell parameters with the temperature.

Conclusions

Tin based architecture for perovskite solar cells are simulated using the SCAPS-1D. The thickness of absorber layer was changed from 0.5µm to 4.5µm for Cu$_2$O, from 0.05µm to 0.250µm for ZnO and thickness for CH$_3$NH$_3$SnI$_3$ from 0.03 µm to 0.07 µm the good performance of a device is achieved at the thickness of 0.03 µm hence the optimum efficiency at thickness 0.03 µm is 8.24%. increasing the defects in the absorber layer and improving the material quality, the device performance will be increased and the minimum defect density for the good efficiency was 10$^{17}$ cm$^{-3}$. The operating temperature was changed from 333.15 K to 233.15K to observe the changes in the PV parameters of the device. The simulation demonstrates that the CH$_3$NH$_3$SnI$_3$, attain a PCE of 9.27%.

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