Using low cost materials for highly efficient eco-friendly FASnI₃ based solar cell with Cu₂O as HTM and TiO₂ as ETM with different metal contacts

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Abstract

Perovskite materials are considered the mainstay of PV manufacturing as outstanding to notable optoelectronic properties. In this work the act of Pb-free FASnI₃ based PSC, TiO₂ as ETL, and Cu₂O as HTL and Ag, Au, Pt, are the different metal contact is simulated using SCAPS software. Here we focused on the impact parameters of device such as the thickness of the Ab-Layer, doping level of perovskite layer and different working temperature. Additionally, we investigated the effect of different metal contact and their work function. The simulated results show that a perovskite layer thickness of 350nm for good perovskite solar cell. For optimizing parameters, efficiency 18.10%, FF 78.14, Jsc 29.61, and Voc 0.7821 have been achieved for Cu₂O and TiO₂ respectively. The thermal study shows that device configurations for this present work at 300k it is stable for this entire work.

1. Introduction

In 1839 Gustav Rose Russian scientist discovered CaTiO₂, and further research was carried by Perovski for that reason scientists called that mineral perovskite. The mineral CaTiO₃ (XIIA₂ + VIB₄ + X₂₋₃) called as perovskite structure [1,15,16]. It is also one of the topmost research in superconductivity, magnetoresistance, conductivity of ions, and Dielectric properties which are significant in telecommunication and others. Perovskite, it is a semiconductor, which is used to transport the electric charge when lights hits the materials. In Oxford University the United Kingdom researchers had found that perovskite has been the instantaneous replacement for third-generation solar cells [2].

Miyasaka has been prepared the first perovskite solar cell in 2009 on DSSC with TiO₂. The PCE is only 3.8% and the stability was very low in the presence of liquid electrolyte. By using a parallel concept park has been enhanced cell efficiency by 6.5% in 2011 by using Quantum dots for monocrystalline materials. In the year 2012 Henery et al. achieve 10% [3], Burschka et al. attain 15 % in the year 2013, Yang Yang is achieving 19.1% PCE in 2014. In the year of march 2016 researchers from the KUST reached 22.1%, In 2020 UNIST reported that they reached 25.5% [4]. However, due to the toxicity of lead, FASnI₃ is an instant alternate material for PSC. Moreover, FASnI₃ has a lower E_g around 1.2 to 1.4 eV, an Ab-coefficient around 105 and excellent optical properties sideways with small effective mass and high mobility (Leet al. 2012, Iefanova, et al. 2016, Anwar, et al. 2017). It has attained 7.13% efficiency, which is considerably low to its Pb-based counterpart (Li, et al. 2019). Because of low-efficiency FASnI₃ is susceptible to the atmosphere due to simplistic oxidation and forms environmentally benign Sn₄₊ from Sn₂₊. From this simulation, aim to forecast the best possible efficiency of FTO/ CuO/ FASnI₃/ TiO₂/ gold (Au) solar cell by optimally varying the thickness, N_d, valence band (VB) effective density of state of the absorber and metal work are calculated. In this paper we attain

18.10 efficiency of FASnI3 based solar cell and also we also signifying CuO2 as a good substitute HTL because of its low cost fabrications and outstanding mobility.

2. Device simulation and structure

In this work, a numerical simulation of a planar heterojunction Sn-PSC was made using SCAPS. FF, Voc, Jsc, PEC, and QE are obtained for this device. The working simulation software is based on 1D. These curves are used to calculate Jsc, Voc, FF, and PCE for this designed solar cell. In this software perovskite solar cells could be designed with several layers, and the simulations done in both mode, In this present work which performed under 1.5G illumination in SCAPS1D design by the University of Gent, Belgium [5,17].

The Device constructs FTO/TiO2/FASnI3/CuO2/metal contact. In this cell structure, FASnI3 acts like light-collecting materials, sandwiched between the ETL (TiO2) and HTL as CuO2. However, FTO is the front contact, and Ag, Au, Cu, Pt were used as a metal contact.

2.1. Methodology of SCAPS simulation

The initial parameters are got from several experimental and theoretical papers are shown in Table 1. The thickness of ETL, HTL, and perovskite layer used in this study are optimized and summarized in table 1. From figure 1. Show the device design configuration of the present work. Through on action panel, we set the parameters and other things for the present work it shows in figure 2. In figure 3. This shows that the device setup panel, in this panel we the thickness, acceptor, donor, and important parameter for the cell.

3. Result and Discussion:

3.1. Impact in the absorbing layer The simulation was done by the basic parameters are tabulated in Tables 1, 2, 3. The impact of the absorber, HTL, ETL are very important things in PSC and reported literature values are needed parameters like PCE%, FF%, Jsc, and Voc [6,18,19]. The variation in the ab-layer thickness from 100-550 nm is shown in this paper. Effect of absorbing layer thickness performance cell configuration Glass/HTL/PEROVSKITE LAYER/HTL/METAL CONTACT is analyzed by changing the thickness of ab-material from 100-550 nm the optimized performance is absorbed in 350nm. The observed details are shown in the figure. 1.

The resultant details are Voc, Jsc, FF, PCE is (0.875-0.753) v, (19.34-31.63) mA/cm², (79.86-72.53) %, respectively we increase the thickness of the ab-layer increase from 100-550 nm for that the above result is voltage decreases, the current density will be increase, Fill factor would be slightly decreased and efficiency are gradually increase and it attains 18.10%. These results are shown in Figures 4 and 5.

The PCE with the thickness of the ab-layer could be explained the basic things like voltage are decrease, the current density would be increase [7,20,21]. It confirms the result data at 350nm thickness of FASnI3 archive 18.10% in this present work device are shown in figure 5.

3.2. Effect of change in Thickness of the HTL and ETL layers

In this work, we have done a lot of trial methods and we attain Cu2O at 400 nm and TiO2 at 100nm thickness of the ETL and HTL layer are respectively. The variations in HTL thickness (100-400 nm) and shown in figure 5 (Voc, Jsc, FF%, PCE%). The resultant details are as follows, the Voc (0.783-0.782)V slightly decreased, Jsc (29.63-29.37) mA/cm² slightly decreased, (76.44-78.55) FF% increased, for that reason the device attains 18.00 % of PCE. The observed getting results are shown in figure 5(a). Simultaneously we change the thickness of the ETL the observer result are given and shown in 5(b).

Now we improve the act data over the absorber layer is different at the adjusted thickness of ETL (100nm). The simulation work for TiO2 (ETL) are taken from 100-350 nm and we confirm 100nm thickness of ETL layer is good for our present work through the results obtained. We construct the cell device for our present work the obtain results are Voc (0.782), Jsc (29.55) mA/cm², FF (78.14%) and the PCE is 18.06%.

3.3. Defect density and doping impacts on the absorber layer

According to SRH recombination supervised the present FA-based device. It is essentially caused by huge defect density due to compact film features [8, 9, 25,]. This type of recombination, carriers in the bands are recombined respectively. Zeetal. [10, 11], the diffusion and less recombination are spotted with an increase in carriers lifetime and a decrease in defect density. This is the hint to advance PSC for this present work. For the proper doping metallic ion, Kang et.al reported [12, 26, and 27]. Variation of defect density ($1\text{E}+12 - 1\text{E}+20$) for the absorber materials. The resultant parameter is observed J_{sc} (29.61 mA/cm^2), V_{oc} (0.7821 V), Fill Factor (78.14%) are slight increases but the important and crucial parameter is PCE 18.10% has been obtained the concentration of defect density at 10^{20} in the absorber. The observed result is shown in figure 6.

Doping is a very effect on the acting data. It can't ever be reduced when the reaction is in the process since the doping may not be the applied process. In this case tin-based cell the oxidation of Sn-2 is detected due to air [13, 14, 22, 23]. If we increase the doping there are two possible things one is an interface and the other one is inside the layers. As per the result, these mechanism increase in the recombination of the carriers at this present work, we put the different the doping value ($10^{12} - 10^{18}$) of the absorber and the obtained result is 18.10% are attained the resultant details are shown in figure 7.

3.4. Consequence of the back work function and the act of PSC

The variations show in the cell configuration CuO as HTL and TiO_2 as ETL and Au as metal contacts are shown in figure 8. The difference of V_{oc} , J_{sc} , Fill factor, and PCE of the FASnI₃ constructed PSC with CuO as HTL and TiO_2 as ETL is shown in figure 9. For different metal contact. The V_{oc} increase with metal work function Au, Cu, Ag, Pt and we attain high efficiency at Au design cell. FF and J_{sc} are also verified for the constructed cell.

3.5. Effect of temperature

At present work study, the temperature of the enhanced device is different from (300-400K) to know the impact of the temperature on this device. The results thus obtained is shown in figure 10. From the results obtained, we observe that the efficiency of the device gradually decreases when increasing the temperature. It might be owing to the point of defect density within the ab layer increasing the temperature for that reason the efficiency of the Sn-based material has been decreased. The observed resultant data are shown in fig. 10 as below

4. Conclusion

In this work, lead-free FASnI₃ based perovskite solar cell was improved and considered for superior PCE by simulation software. The impact of the difference in Thickness of HTL, ETL, and Ab layer on PCE was studied, and the thickness of 400nm, 100nm, 350nm were obtained respectively. The outcome of the difference in defect density and acceptor was also considered and improved. We done our present work in same method for all and finally we attained the PCE is 18.10% along with J_{sc} (29.61 v), FF (78.14%), V_{oc} (0.7821 v), which are a dynamic section for an enhanced perovskite solar cell. The device performance with the stable temperature at 300K. Through a back metal contact Au with work function 5.1 eV . The QE of the improved solar cell remains constant till 580nm then drop to zero at 910nm, showing that the photon to electron conversion occurs over the visible region as shown in figure 11(a),(b). Results are also compared with already reported experimental and simulation data. Finally, we got 18.10% of PCE. So here we proposed a novel simulation model replacing the pb-based PSC with Sn based FASnI₃ to study its performance, and also suggesting CuO₂ as an alternate HTL because of its low cost fabrications and outstanding mobility.

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