



PERFORMANCE ANALYSIS OF PEROVSKITE SOLAR CELL WITH ALL INORGANIC HOLE TRANSPORT AND ELECTRON TRANSPORT LAYERS

Md. Samiul Islam Sadek, Mst. Sarmin Aktar, Md. Foyisal Kabir Shimul and Md Ashraful Islam

Abstract—Inorganic metal halide Perovskite solar cells are becoming the leading alternative for the traditional Si-based solar cells not only for its unprecedented power conversion efficiency (PCE) (~22.1%), but also for their superior electrical and optical properties. However, due to the lack of proper understanding of its structural and electric-chemical characteristics, the PCE is still lagging behind some existing photovoltaic technologies. Therefore, a detailed understanding of the function of the various constituent layers of this solar cell's planar architecture is still necessary to verify the overall efficiency. In this research paper, a planar hetero-structure based perovskite solar cell along with all inorganic transport layers are simulated to examine the performance of the cell under the varying thicknesses and doping concentration of various layers. The measured performance parameters are open circuit voltage (V_{oc}) and short circuit current (J_{sc}), Fill Factor (FF) and Efficiency (η). It has been identified that the thicknesses of the different layers specially, perovskite absorber and TiO_2 have significant impact on the performance of the cell. It has also been found that, performance of the cell alters with the variation of doping concentration of both Electron Transport Material (ETM) and Hole Transport Material (HTM) as well.

Keywords—Solar Cell, Perovskite, Inorganic, Transport Material, Transport Layer, Thickness, Concentration.

I. INTRODUCTION

IN the low temperature and solution manufactured solar cells have been reformed by hybrid organic-inorganic metal halide perovskite materials over the

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last few years, demonstrating the power conversion efficiencies (PCEs) that compete with the undisputed decades-old matured silicon-based PV technologies. Till now, extensive studies on perovskite solar cells (PSCs) centered on polycrystalline film and the recorded efficiency is ~24.2 % [1], which still lag from the theoretical Shockley- Queasier Limit (SQL), which is ~30.5% PCE for a single junction cell based on Methylammonium Lead Iodide ($MAPbI_3$). The PSCs' lifetime may be enhanced by tuning different parts of the device and its constituents [2]: perovskite crystal structure, cell encapsulation, film quality, alternative designs, conducting layers and interfaces. The perovskite solar cell (PSC) has generated motivation in scientific research as a capable third-generation solar cell (SC) with a significant increase in power conversion efficiency from 3.8 percent in 2009 [3] to more than 22 percent in 2017 [4-6]. The simpler planar arrangement has been often selected as the PSC structure compared to a porous scaffold pattern [7-8]. A hetero junction architecture with three main layers, i.e. electron transport material (ETM), perovskite absorber, and hole transport material (HTM), usually contains the planar PSC.

Generally, the morphology control of perovskite films using novel materials, the optimization of the device structure, the alternative HTM layer and the growth of effective manufacturing methods are crucial factors for the production of competent planar PSCs [4-6]. TiO_2 or ZnO has been used as an ETL [9-12] and 2,2,7,7-Tetrakis (N,N-di-4-methoxyphenylamino)-9,9'-Spirobifluorene (commonly referred to as spiro-MeOTAD) so far been the only major option as an HTL, so that holes have faced no energy barrier at the $MAPbI_3$ /HTL and HTL/gold interfaces [11-13]. The pristine Spiro-MeOTAD has a low mobility hole and a low concentration of acceptors [14]. In order to substitute spiro-MeOTAD with a more stable and less costly suitable material, such as CuI [9], $CuSCN$ [10], [15-16] or copper phthalocyanine [17], an alternative is therefore needed.

In this research, we have concentrated on inorganic hole transporting materials (HTMs), to enhance the

power conversion efficiency (PCE) by reducing recombination current of solar cell as HTM consumes hole from absorber that decreases electron-hole recombination into the absorber. The good performance of such perovskite solar cells can be attributed to the unique properties of ultra-thin Cu_2O , including high holes mobility, good energy level alignment with $\text{CH}_3\text{NH}_3\text{PbI}_3$, and extended lifetime of photo-excited carriers. Cu_2O films, generated by thermal oxidation, combine the merits of low cost, easy synthesis and high system performance to facilitate the growth of industrial-scale perovskite solar cells. There are some outstanding reasons for using Cu_2O as the hole transport layer. Copper-based materials have higher charge mobility and high current density as compared to spiro-OMeTAD having smaller molecular size and higher weight of molecules. Moreover, Metal oxides enjoy long term durability because of their environment friendly nature. Because of its narrower band gap, the copper oxide layer absorbs more lights incident on it.

II. METHODOLOGY

In addition to the experimental study, the simulation provides a powerful means to better realize about the physical behavior of different electrical and optical characteristics of the proposed solar cell. In relation to the electrical simulation, the software like the Solar Cell Capacitance Simulator (SCAPS-1D) [18] basically works on three basic semiconductor equations such as, the Poisson equation and the continuity equation of electrons and holes under steady-state condition.

SCAPS-1D describes a solar cell as a series of layers with different opto-electrical properties as well as defect states of each layer and interface. It is well adapted for the analyses of homo and hetero junctions, multi-junctions and Schottky barrier photovoltaic devices, such as micro and Polly-crystalline thin film devices [5-6], [19]. According to options of these 1D codes such as SCAPS, most of these studies focus more on various factors such as layer thickness, working temperature, illumination intensity, different solid-state parameters of layers (mobility, band gap, doping type/concentration, etc.) Therefore, they investigated the influence of these factors on the basic parameters of the solar cell (FF, V_{OC} , J_{SC} , and PCE). This reference provides a comprehensive study in this regard [19]. In this respect, proper modeling of the absorption layer is of great importance, especially for the simulation of the External Quantum Efficiency (EQE) spectrum.

III. DEVICE ARCHITECTURE

The most widely exploited $\text{CH}_3\text{NH}_3\text{PbI}_3$ is used as the main absorber material sandwiched between two transport layers in an inverted planar hetero-structure. In such a structure, TiO_2 is used as the electron transport

layer material due to its special electrical and optical properties. The typical holes transport material is replaced by the inorganic Cu_2O material. The schematic diagram of the device structure is shown in Fig. 1.

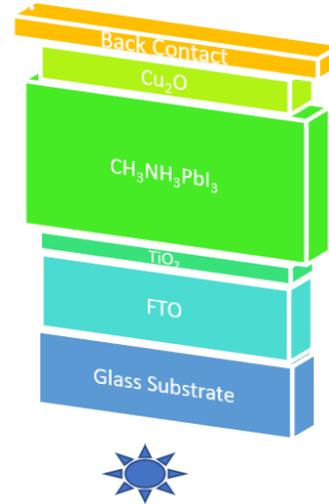


Fig. 1. Architecture of the device

The material parameters used in this work are shown in the following Table 1.

TABLE I
INPUT PARAMETERS OF DIFFERENT CONSTITUENT LAYERS
FORMING THE SOLAR CELL

Parameter	FTO	TiO ₂	CH ₃ NH ₃ PbI ₃	Cu ₂ O
Thickness (m)	0.4	0.05	0.45	0.15
Energy gap (E_g)	3.5	3.26	1.55	2.17
Electron affinity (χ)	4	4.2	3.9	3.2
Dielectric Constant (ϵ)	9	10	6.5	11.9
Density of states in CB (cm^{-3})	2.2E+18	2.2E+18	2.5E+18	2.2E+18
Density of states in VB (cm^{-3})	1.8E+18	1.78E+18	1.8E+18	2.2E+18
Electron mobility (μ_n) ($\text{cm}^2/\text{V.s}$)	2.0E+1	2.0E+1	2.0E+1	8.0E+1
Hole mobility (μ_p) ($\text{cm}^2/\text{V.s}$)	1.0E+1	1.0E+1	2.0E+1	8.0E+1
Acceptor concentration (N_D) (cm^{-3})	1.0E+19	1.0E+17	0	0
Donor concentration (N_A) (cm^{-3})	0	0	1.0E+13	1.0E+18

IV. RESULTS AND DISCUSSIONS

A. Effect of absorber layer thickness and acceptor doping concentration

The thickness and carrier concentration of the perovskite absorber layer is varied from 0.2 to 1.0 μm and doping concentration from $1\text{E}13 \text{ cm}^{-3}$ to $1\text{E}18 \text{ cm}^{-3}$ respectively. During the thickness variation, the acceptor doping concentration of absorber was fixed at $1\text{E}15 \text{ cm}^{-3}$. Similarly, thickness of absorber was



optimized at 0.6 μm while examining the concentration of the absorber. The remarkable changes found from the simulation results shown in Fig. 2.

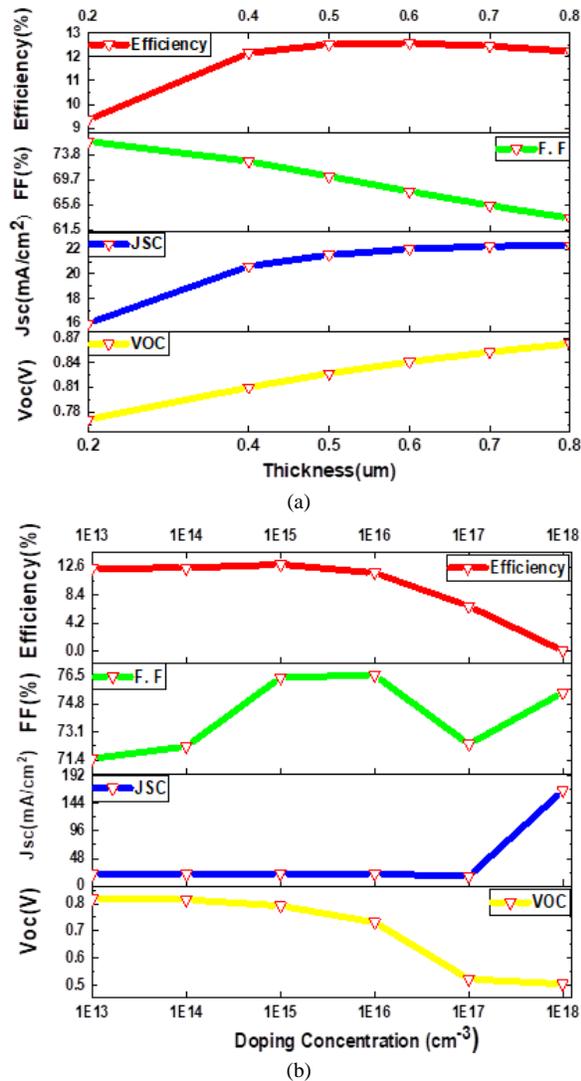


Fig. 2. (a) Effects of the thickness and (b) acceptor doping concentration of perovskite (absorber) layer

It is clear from the Fig. 2 (a) that the optimum thickness of the perovskite layer is about 500 nm, because the efficiency falls down in either sides of this optimum thickness. In case of lower thickness, the most of the incoming sunlight are transmitted rather than absorbed. So, less number of electrons and holes are produced, which eventually reduces the efficiency. On the other hand, too much thick absorber increases the chances of recombination. So, collection efficiency gets reduced.

Moreover, it is clear from the Fig. 2 (b) that the optimum acceptor doping concentration was $1\text{E}1015$ cm^{-3} , because the efficiency and fill factor falls down

further increased acceptor doping concentration beyond optimum acceptor doping concentration. Increasing acceptor doping concentration means higher values of short circuit current (J_{sc}), but the open circuit voltage (V_{oc}) decreases beyond $1\text{E}15\text{cm}^{-3}$. The reason is higher values of doping concentration decreases the distance between the quasi-Fermi level, which is eventually related to the open circuit voltage.

B. Thickness and donor doping concentration variation of TiO_2 layer

The Electron transport layer plays a vital role in isolating the photo generated carrier in the absorber layer. This layer should be sufficiently narrow in order to pass the photon to the absorber layer. In this work, the thickness of this layer is varied from 10 nm to 100 nm keeping the donor concentration of TiO_2 at $1\text{E}17$ cm^{-3} .

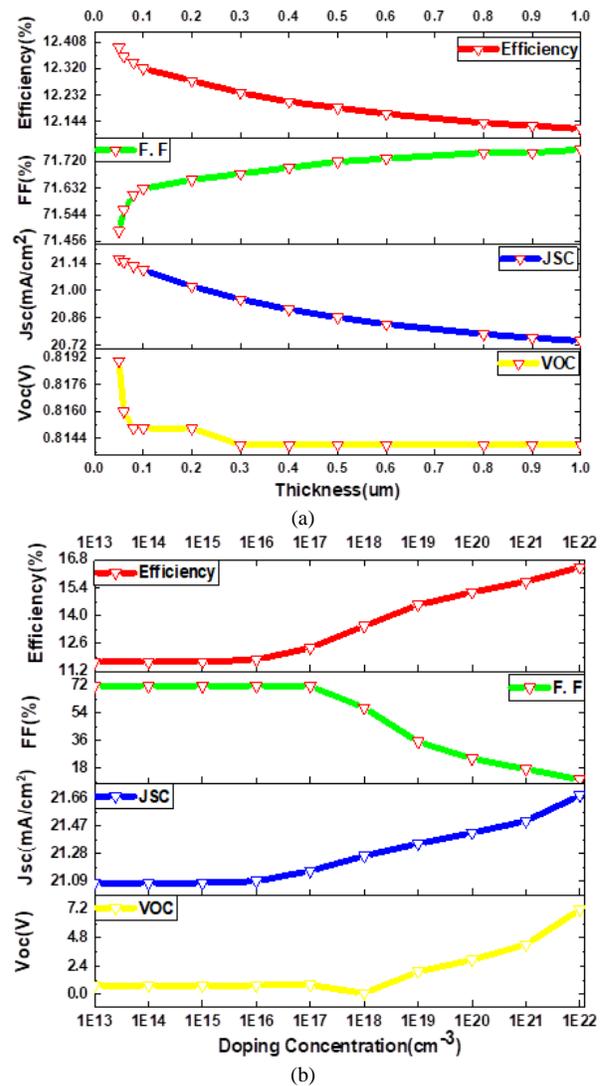


Fig. 3. (a) Effects of the thickness and (b) Donor doping concentration of TiO_2 layer (electron transport layer)

It has been depicted from the Fig. 3 (a) that the efficiency gradually decreases as the thickness increases because, higher the thickness means maximum incoming light will be absorbed in the electron transport layer rather than reaching through the absorber layer. The highest efficiency is achieved at around 10 nm, but this value is optimized to 50 nm for sake of practical feasibility and the variation of doping concentration is performed on that fixed 50 nm thickness. It has been also observed from Fig. 3 (b) that there is a sharp fall in open circuit voltage at the concentration level of $1E17 \text{ cm}^{-3}$ and there is a gradual increase of short circuit current and efficiency as well. This is obvious because, if the doping concentration increases, no of carriers will increase, so short circuit current will increase. Therefore the optimum thickness and donor doping concentration of TiO_2 layer is chosen $0.05 \mu\text{m}$ and $1E17 \text{ cm}^{-3}$ respectively.

C. Thickness and acceptor doping concentration variation of Cu_2O layer

From Fig. 4 (a), there is apparently no change in the performance parameters due to increase of thickness of the hole transport layer, but from Fig. 4 (b), we can see that doping concentration of Cu_2O layer seems to have a significant impact on the performance of the cell. It is obvious because the hole transport layer is the layer which facilitates the hole to move to the back contact of the cell without interrupting the light absorption. As per short circuit current and the efficiency is concerned, the optimum doping concentration is about $1E17 \text{ cm}^{-3}$ or $1E18 \text{ cm}^{-3}$ or so. The noteworthy point is all the measured parameters become saturated after reaching the above-mentioned range of doping concentration.

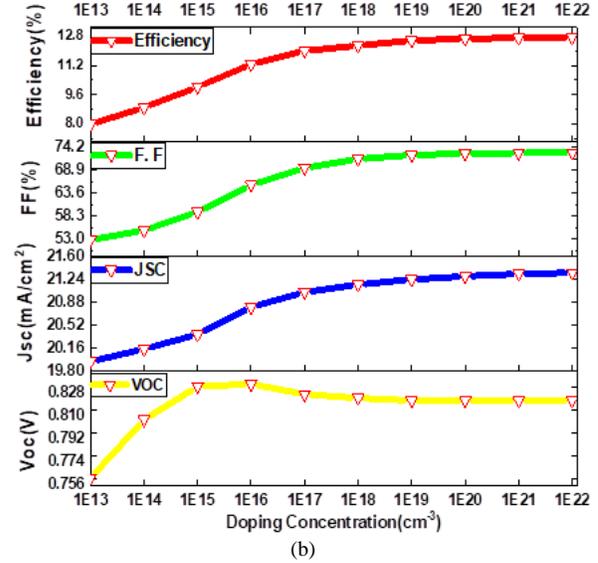
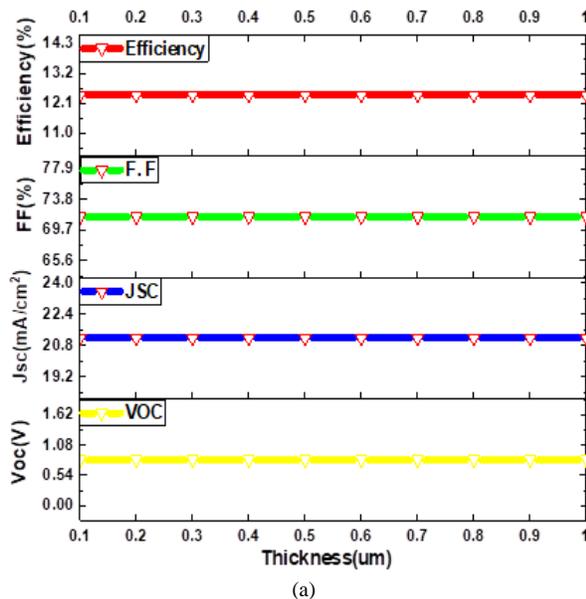


Fig. 4. (a) Effects of the thickness and (b) Acceptor doping concentration of Cu_2O layer (holes transport layer)

D. Defect density variation of Cu_2O layer

The performance variation due to various defect values are also examined, which is shown in Fig. 5.

The defects are one of the basic parameters which hinder the performance of a solar cell as a whole. This defect actually acts like a trap state or recombination center for the photo generated carrier while travelling through the device. The material having higher defect densities should exhibit the fall in short circuit current as well as the efficiencies. The outcome of the simulation shows the exact thing. Here both short circuit current and efficiency decreases very sharply when the defect densities reach beyond $1E15 \text{ cm}^{-3}$.

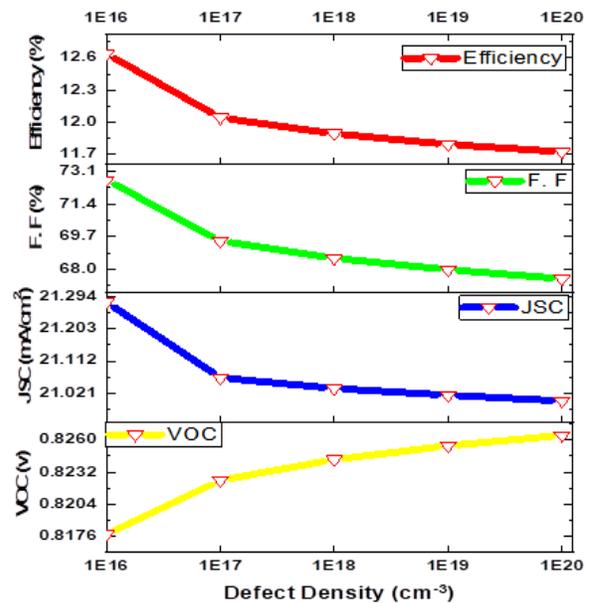


Fig. 5. Effect of defect densities of Cu_2O layer



V. CONCLUSION

In this research, all inorganic transport layers are employed to test the performance of the perovskite solar cell. It has been revealed from the simulation results that, the thickness of the absorber material is the most important parameters to obtain the higher efficiency. As $\text{CH}_3\text{NH}_3\text{PbI}_3$ has ambipolar characteristics, so variation of doping concentration is not the defining parameters. But in case of electron transport and holes transport layer material, both thickness and concentration are equally important. It has been found that, the TiO_2 thickness about 20 nm gives the maximum efficiency and doping concentration should not exceed $1\text{E}18\text{ cm}^{-3}$. In case of holes transport layer, the defects play a significant rule rather than the thickness and concentration.

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