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MODELING OF EFFICIENT PEROVSKITE SOLAR CELL WITH DOUBLE ABSORBER LAYERS

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Abstract- *Organo-metal halide Perovskite solar cells based on lead halide Perovskites having large absorption coefficient, high carrier mobility and superb photovoltaic performance achieved high power conversion efficiency with low cost. In this work, two different high performance Perovskite solar cells were designed and simulated using WXMPS. One cell with single absorber layer ($CH_3NH_3PbI_3$) achieved a high PCE of 22.21%, Voc=0.992V, Jsc=26.05mA/cm2 and FF=85.89%. Another cell using two absorber layers ($CH_3NH_3PbI_3$ and $CH_3NH_3PbBr_3$) achieved a PCE of 23.32%,* Voc *= 0.993V, Jsc = 27.99mA/cm2 and FF = 83.85%. The power conversion efficiency is greatly dependent on the thickness of Perovskite layers. By varying the thickness of the absorber layer the performance of solar cell is checked.*

Keywords: Organometal halide perovskites solar cells, $CH_3NH_3PbI_3$, $CH_3NH_3PbBr_3$, power conversion efficiency.

1. INTRODUCTION

Day by day demand for power is increasing, but the energy source for generating power such as coal, natural gas, oil etc. are limited. So in the near future we have to rely on the renewable energy. Solar energy is one of the reliable sources of renewable energy. If we can use the solar energy for producing electricity with low cost, the energy crisis problem can be solved. Perovskite is a new material used in solar cell as a light absorber and these type of solar cells are cost effective and their efficiency is increasing rapidly.

A Perovskite is a material with the same type of crystal structure as calcium titanium oxide ($CaTiO_3$), known as the Perovskite structure as XIIA2+VIB4+X2−3 [1]. Perovskites take their name from the mineral, which was first discovered in the ural mountains of Russia by Gustav Rose in 1839 and is named after Russian mineralogist L. A. Perovski (1792–1856). The basic structure of Perovskite compounds is ABX_3, where A, B are cations and X is anion. Cation A is greater than cation B. Mostly used Perovskite for solar cell are formed with methyl ammonium as cation A, Pb as cation B and helogen as X respectively. The 3D structure of ABX_3 is shown in Fig. 1. The PCE of Perovskite solar cells is increasing rapidly and this rapid development could be achieved because of advantageous characteristics of Perovskite materials which include an appropriate direct band gap, a high extinction coefficient, long diffusion length and good tolerance of defects [3-4].

The structure of the employed device here is a p-i-n solar cell where ZnO is used as n-type and Cu_2O is used as p-type material.

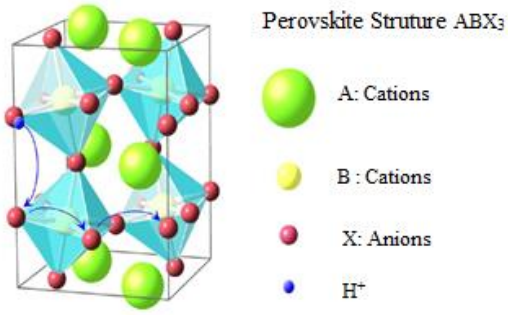

Fig. 1. 3D Structure of Perovskite material [2].

Perovskite-based hybrid organic halide materials are not new materials and have been extensively studied because of their useful physical properties, including enhanced binding energies, nonlinear optical properties, electroluminescence, organic-like mobility, magnetic properties, and conductivity [8-13]. Perovskite materials are used in solar cells since 2009. Scientists of Toin University of Yokohama firstly started working on Perovskite in 2009. The first Perovskite-sensitized TiO_2 solar cell used liquid electrolytes based on iodide and bromide. The corresponding devices gave PCEs of 3.8% and 3.1%, respectively [14]. Later, in 2012, when Henry Saith and Mike Lee from the University of Oxford showed that efficiencies of almost 10% were achievable using the 'sensitized' TiO_2 architecture with the solid-state hole transporter. In 2013 both the planar and sensitized architectures saw a number of developments. Burschka et al. demonstrated a deposition technique for the sensitized architecture exceeding 15% efficiency by a two-step solution processing [15]. Meanwhile, a simple

planar-heterojunction (p-i-n) solar cell incorporating vapor-deposited Perovskite as the absorbing layer has been developed, and demonstrated a solar-to-electrical PCE of 15.4% [16]. A range of new deposition techniques and even higher efficiencies were reported in 2014. A reverse-scan efficiency of 19.3% was claimed by Yang Yang at UCLA using the planar thin-film architecture [17]. In November 2014, a device by researchers from KRICT achieved a record with the certification of a non-stabilized efficiency of 20.1%. In December 2015, a new record efficiency of 21.0% was achieved by researchers at EPFL. The newest record of efficiency have been increased to 22.1% at KRICT/UNIST [18].

As intrinsic layer $CH_3NH_3PbI_3$ and $CH_3NH_3PbBr_3$ are used. The p-type Cu_2O has good transparency, high hole mobility and good chemical stability. Also it is nontoxic and abundantly available on the earth. By adjusting the thickness of Perovskite layers, the PCE of the cell can be improved.

The Perovskite solar cells with spiro-OMeTAD as p-type material have achieved high PCEs of about 20%. However, the synthesis of spiro-OMeTAD becomes a barrier for future commercialization because of its high cost. So it is necessary to use other p-type materials as a substitute for spiro-OMeTAD [5]. Compared with organic spiro-OMeTAD, inorganic p-type Cu_2O with similar physical property, good chemical stability, ease of synthesis procedure, and low cost is an ideal kind of p-type material. ZnO has an energy-band structure and physical properties similar to those of TiO_2. But ZnO has substantially higher electron mobility than that of TiO_2, which would make it an ideal kind of n-type material [6-7]. Therefore, Cu_2O as HTM and ZnO as ETM are widely utilized to Perovskite solar cells. To achieve higher efficiency with Perovskite solar cell, it is important to study the effect of the Perovskite material, transport materials and device architecture on device performance. In this paper, the effects of the material thickness and material properties on device performance are investigated to help further effort toward high-performance Perovskite solar cells.

2. DESIGN OF PEROVSKITE CELL

Two different Perovskite solar cells are designed to simulate the effects of architectures and material properties on the device performance. The solar cell with a Perovskite layer ($CH_3NH_3PbI_3$) sandwiched between ZnO and Cu_2O is shown in Fig. 2(a). Secondly, the designed solar cell with double light absorbers with both $CH_3NH_3PbI_3$ and $CH_3NH_3PbBr_3$ which are intrinsic is shown in Fig. 2(b). The two devices $CH_3NH_3PbI_3$ ($MAPbI_3$) and $CH_3NH_3PbBr_3$ ($MAPbBr_3$) have their own characteristics: high PCE and *Jsc* for $MAPbI_3$, and high V_{oc} for $MAPbBr_3$. Thus for structure with $CH_3NH_3PbI_3$ we get high *Jsc* and high power conversion efficiency and for $CH_3NH_3PbBr_3$ we get high V_{oc} These characteristics of two Perovskites (CH3NH3PbI3 and CH3NH3PbBr3) are combined in structure of Fig. 2(b) to get high PCE and Jsc as well as high Voc which results in overall higher efficiency.

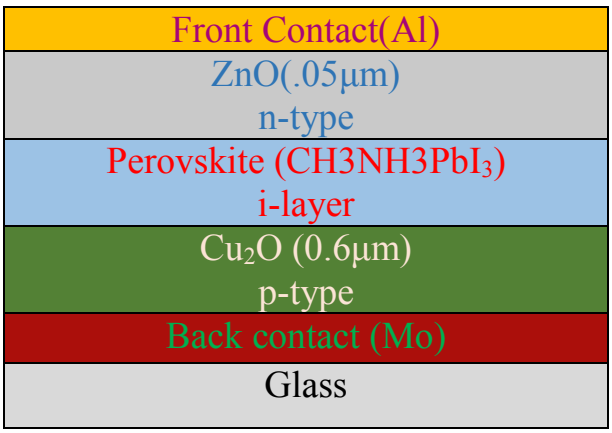

Fig. 2(a). Proposed structure of a Perovskite solar cell with an absorber layer of CH3NH3PbI3.

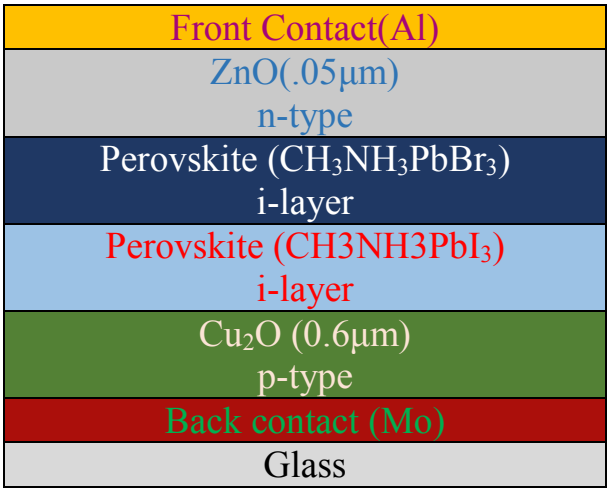

Fig. 2(b). Proposed Structure of a Perovskite solar cell with two absorber layers of CH3NH3PbBr3 and CH3NH3PbI3.

3. SIMULATION METHOD

To simulate the cells we used a simulation software named WXMPS. The WXMPS program is a newly developed solar cell simulation software based on the original AMPS (Analysis of Microelectronic and Photonic Structures) code [19]. The WXMPS software incorporates two different tunneling models for better simulation of specific types of solar cells. The intra-band tunneling model provides more realistic characteristics for heterojunction solar cells compared to the drift-diffusion model. To increase the convergence property of the intra-band tunneling model, a new algorithm that combines the Newton method and the Gummel method has been developed. The simulation results from different models are compared [20].

4. RESULT AND DISCUSSION

In this section we analyze the performance of the two structures in Fig. 2(a) and in Fig. 2(b) using WXAMPS under AM1.5 illumination. The physical parameters of the solar cell has been taken from table 1.The highest efficiency was recorded via changing thickness and keeping it under optimum limit. The single junction Perovskite solar cell is simulated and the output J-V characteristic curve is plotted in fig. 3.

Table 1. Properties of materials used in designed cell.

Properties	ZnO (n-type)	$MAPbB_3$ (i-layer)	$MAPbI_3$ (i-layer)	Cu_2O (p-type)
Thickness	0.05	15	15	0.7
Bandgap (eV)	10	30	30	7.5
Electron affinity (eV)	3.37	1.95	1.5	2.22
Dielectric Permittiviy (relative)	4.35	3.93	3.93	3.6
CB effective density of states (cm^{-3})	$2.22x10^{18}$	$2.5x10^{20}$	$2.5x10^{20}$	$1x10^{19}$
VB effective density of states (cm^{-3})	$1.78x10^{19}$	$2.5x10^{20}$	$2.5x10^{20}$	$1x10^{19}$
Electron mobility (cm^2/Vs)	100	14	50	30
Hole mobility (cm^2/Vs)	25	14	50	30
Donor Concentration (cm^{-3})	$1x10^{18}$	0	0	0
Acceptor Concentration (cm^{-3})	0	0	0	$1.5x10^{15}$

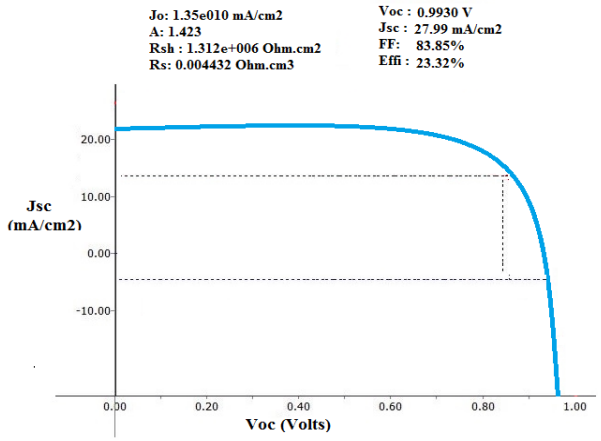

Fig. 3. J-V Characteristics of single junction Perovskite cell in wx-AMPS in AM 1.5G.

From the J-V characteristic curve we got an efficiency of 21.82%, JSC= 26.5752mA/cm2, Voc = 0.9753V, fill factor = 84.3424% for single junction Perovskite cell (Fig.2).

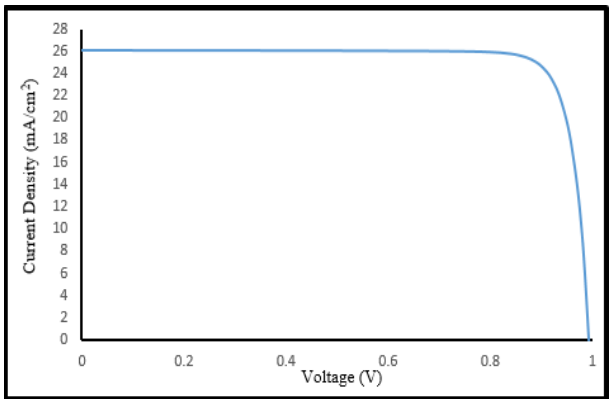

Fig. 3(a). J-V characteristics of Perovskite solar cell for the $Mo/Cu_2O/MAPbI_3/ZnO/Al$ architecture simulated with thickness of $MAPbI_3$ = 15µm.

From the simulation of the structure of $Mo/Cu_2O/MAPbI_3/ZnO/Al$ architecture, the J-I characteristics is drawn in Fig. 3(a).When the thickness of $MAPbI_3$ was 15µm, the PCE is 22.21%, Voc=0.992V, Jsc=26.05mA/cm2 and FF=85.89% have been attained from this structure. The thickness is varied to see the effect of the thickness on J-V characteristics as shown in fig 3(b). When the thickness of MAPbI3 is 50nm, current density is 17.61mA/cm2 and when thickness is 15µm, Jsc is 26.05mA/cm2. Thus increasing the thickness of absorber layer increases current density, so PCE also increases with thickness. PCE of the $Mo/Cu_2O/MAPbI_3/ZnO/Al$ structure with varying thickness of MAPbI3 is drawn in Fig. 3(c). It is seen that with the increase of thickness of the intrinsic layer of $MAPbI_3$, the efficiency increases rapidly and after reaching a certain efficiency the PCE slowly increases with thickness. At 10µm thickness of absorber, PCE is 21.48% and then it increases slowly to 22.21% for further increase in thickness for 15µm.

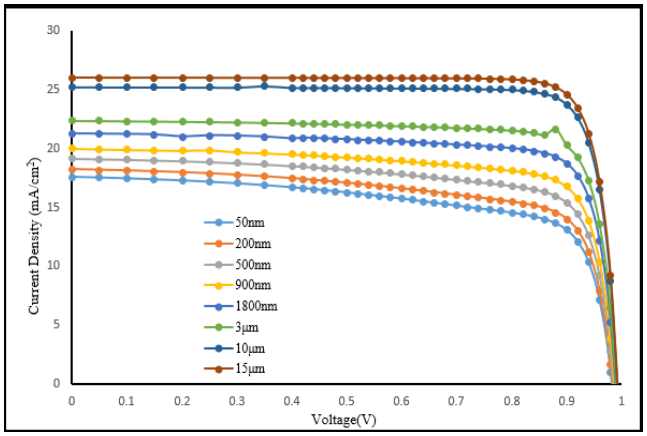

Fig. 3(b). J-V characteristics of Perovskite solar cells for $Mo/Cu_2O/MAPbI_3/ZnO/Al$ architecture simulated with different thickness of $MAPbI_3$.

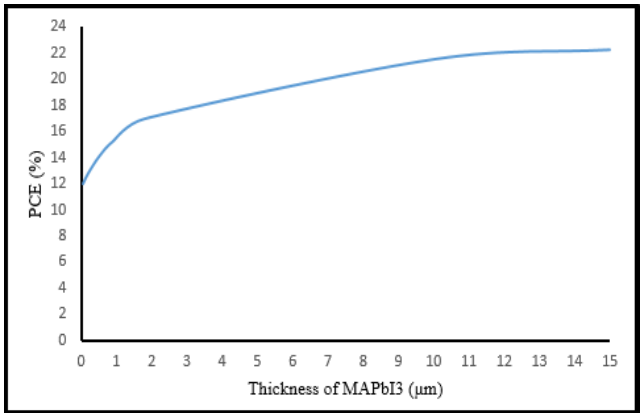

Fig. 3(c). Effect of thickness on PCE of Perovskite solar cell for Mo/Cu2O/MAPbI3/ZnO/Al architecture.

The increase in thickness of $MAPbI_3$ of 5µm increases PCE of just about 0.73%. The J-V characteristics of $Mo/Cu_2O/MAPbI_3/MAPbBr_3/ZnO/Al$ architecture is

shown in Fig 3(d) with thickness of $MAPbI_3$ =15µm and $MAPbBr_3$ =15µm. The simulation results show that PCE is obtained 23.32% (*Voc*=0.993V, *Jsc*=27.99ma/cm^2 and FF=83.85%).

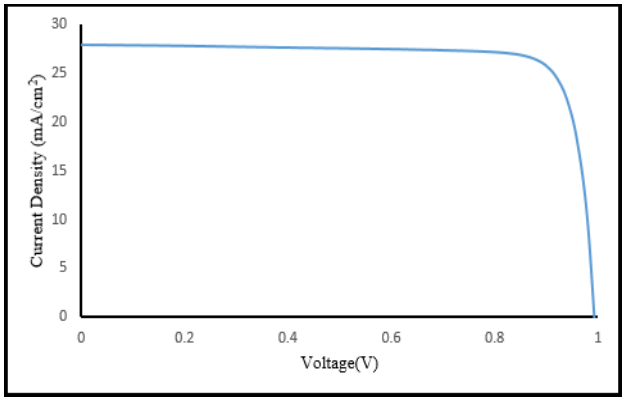

Fig. 3(d). J-V characteristics of Perovskite solar cells for the Mo/Cu_2O/$MAPbI_3$/$MAPbBr_3$/ZnO/Al architecture simulated with thickness of $MAPbI_3$=15µm and $MAPbBr_3$=15µm.

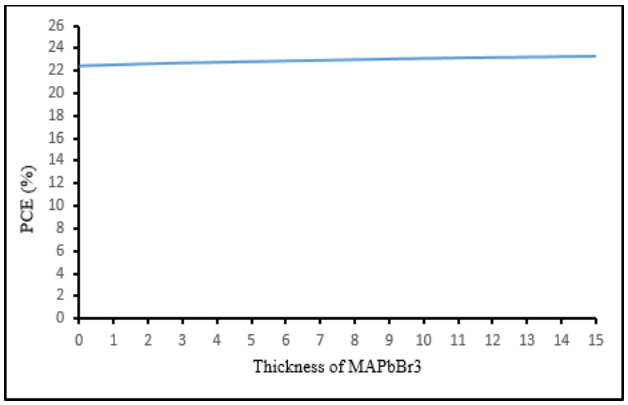

Fig. 3(e): Effect of thickness on PCE of Perovskite solar cell for Mo/Cu_2O/$MAPbI_3$/$MAPbBr_3$/ZnO/Al architecture while thickness of $MAPbBr_3$ is varied with 15µm thickness of $MAPbI_3$.

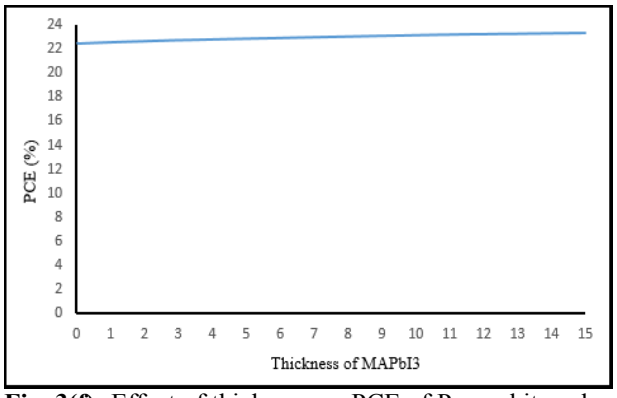

Fig. 3(f): Effect of thickness on PCE of Perovskite solar cell for Mo/Cu2O/$MAPbI_3$/$MAPbBr_3$/ZnO/Al architecture while thickness of $MAPbI_3$ is varied with 15µm thickness of $MAPbBr_3$.

The effect of thickness of $MAPbBr_3$ while fixing the thickness of $MAPbI_3$ as 15µm on PCE is found in Fig. 3(e). As the thickness of $MAPbBr_3$ increases, PCE increases very slowly. At 200nm thickness of $MAPbBr_3$, PCE is 22.42%. Again changing the thickness of MAPbI3 while keeping the thickness of $MAPbBr_3$ as 15µm, the change in PCE is observed in Fig. 3(f). The PCE is firstly decreases with this thickness of $MAPbI_3$ from 20nm to 50nm. At 20nm, PCE is 22.5% and at 50nm, it is 22.46% then slowly increases and finally highest PCE is found at 15µm. As a result, it is observed that by increasing the thickness of absorber layers ($MAPbI_3$ and $MAPbBr_3$) after a certain thickness (approximately 10µm), the increase in PCE is not greater than 1%.

6. CONCLUSION

This paper has been focused on the study of two absorber layers on organometal halide Perovskite based solar cell. We have discussed the outcome of a simulation study on organometal halide Perovskite focusing on the thickness of absorber layer of the solar cell using WXMPS as a simulation tool. A high performance of PCE=23.32%, Voc = 0.993V, *Jsc* = 27.99mA/cm^2 and FF = 83.85% have been observed for double absorber layers of thickness 15µm while with only one absorber layer ($MAPbI_3$) the PCE was 22.21%. The Perovskite solar cell with double light absorbers possess an extraordinary characteristics of PCE and *Jsc* by changing the thickness of $MAPbI_3$ and $MAPbBr_3$.

7. REFERENCES

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