Comparative Analysis for Various Hole Transport Material to study Efficiency Up gradation in Tin Based Perovskite Solar Cell

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Abstract— Perovskite sun based non-toxic cells which have picked up much inquire about eagerness since of the poisonous nature of the lead-based halide perovskite (MASnI3). MASnI3 may be a attainable differentiating alternative to $MAPbX_3$, in light of the truth that it has broader obvious assimilation range run and littler band hole esteem of 1.3 eV than MAPbI3. The progress of manufacturing tin-based PSCs with extraordinary quality has enlivened the examinations of these MASnI3-based sun based cells hugely. In this paper, planar hetero junction plan of Tin-based iodide PSC is proposed. The copper iodide (CuI) which is inorganic material is utilized for the exceptionally to begin with time as gap transport layer (HTL) in conjunction with the MASnI3 dynamic layer in this plan since of its characteristic highlights as compared to the unsteady and exorbitant Spiro-OMeTAD,CuO_2 and copper iodide (CuI) as a hole transport layer, the results are accomplished with short circuit current density (Jsc) of 27.56 mA/cm2, open circuit voltage ($Voc_)$ of 1.08 V, fill factor (FF) of 87.42 and power conversion efficiency (PCE) of 26.10.

Keywords: Non-Toxic Perovskite Solar Cell, HTM, SCAPS, Efficiency, Stability

I. INTRODUCTION

The Perovskites, are a class of compounds named after the Russian mineralogist L.A. Perovski. Perovskite are represented by using the formula ABX_3 where A and B are cations of different sizes and halogen X may be chlorine iodine or bromine ion. The MAPbX3 PSCs have drawn considerable consideration because it has easier methods of formation and lower fetched figure than ordinary Si sun-oriented cells[1]. The efficiency of MAPbX3-based sun powered cells have been significantly enhanced over the past couple of years from 3.80% in 2009 to an estimate of 25.20% in 2020[2]–[5]. Lead toxicity remains a critical barrier to large-scale use of these cells. Speculative and exploratory experiments show that MASnI3 has a littler 1.3eV band gap that can span a broader spectrum of unmistakable spectrum relative to the $MAPbI_3$ band gap(1.55eV)[6][7]. Since Pb-free Sn- dependent perovskite is elective, dynamic layers have been used in cells. Recently, due to developments in encapsulation and production methods, the stability of MASnI3 has been enhanced to a significant degree. There is a major reduction in the Sn4+, with the inclusion of tin SnF_2 in the structure oxidation cycle resulting from Sn2+.[8] This technique is actually commonly applicable to the manufacturing of tin solar cells. As shown by the latest research work, the maximum efficiency reported by different analysts is more than 24 percent. One of the problem relating to these PSCs is the use of expensive Spiro-MeOTAD[9] due to muddled synthesis methods or high-purity preconditions such as HTL. Stability is another concern for long haul use. Subsequently, the use of organic materials as HTL will discourage marketing of sun based cells, after considering workability and cost factors. Having a clear final goal of looking at HTL's conductivity for these solar cells, the choices are the inorganic p type semiconductors due to stability(chemical) and high value of mobility. Such components have a variety of energy levels of valence band[10]. CuI HTL material has been accounted as having a meso-scopic structure in the perovskite cell. Xiamen University researchers presented a 13.58 percent efficiency value for the planar structure using perovskite as an absorbent layer. For these PSCs with efficiencies of 15.4 percent & 12.4 percent, various materials (p-type) such as nickel oxide (NiO_2) and CuScN were used. Considering the impediment in the wealth of substances and hardware, the effect of different hole transport materials on these cells' working is best investigated through modeling processes and various simulation methods.[11] The profound and excellent insight into the enhancement of different cell parameters can be obtained in this manner.[12] One more thing is that it will diminish the chances of producing a low-efficiency solar cell. With the parameters described the research have been conducted a Sn based cell with HTL materials, Spiro-MeOTAD, Cu_2O and CuI. Nevertheless, as an alternative to organic Spiro-MeOTAD, more HTL for solar cells may be suggested. Furthermore, the other researchers examined different materials for solar cell formation. The most bountiful and inexpensive material is copper Iodide, possesses a strong band gap along with compatibility at higher temperature. The perovskite-based solar cell, consisting of glass / transparent con- ducting oxide, buffer layer, perovskite layer, hole transfer medium and back contact layers, was re-engineered in this research.

II. BASIC DEVICE STRUCTURE AND SIMULATION

Typical perovskite solar cell structure consisting of a p-type layer, n-type layer as a carrying medium for electrons, and an absorbent layer sandwiched in between. Such conveyor layers are further achieved by touch (may very various configurations). Dielectric constant selection has several ideas, high value for which excitation can be converted very easily into free carriers[13].

$$D\frac{\partial^2 n(x)}{\partial x^2} + \mu E(x)\frac{\partial n(x)}{\partial x} + G(x) - R(x) = 0 \qquad (1)$$

$$D\frac{\partial^2 p(x)}{\partial x^2} - \mu E(x)\frac{\partial p(x)}{\partial x} + G(x) - R(x) = 0 \qquad (2)$$

For electrons and holes, the above equation (1) and (2) is a steady state continuity equation. Where n(x) and p(x) are concentrations of n and p, G(x) is the rate of photo generation and R(x) is the recombination of the charges. Using the equation within the absorber layer, an analytical model is created. Using these equations the corresponding

values for the parameters are determined. The diffusion constant and carrier mobility are respectively in the equation given above, D and μ. The solar cell that uses tin perovskite as the active layer in a planar design was introduced in this research work. Different layers deployed in this framework include glass / TCO / buffer layer (TiO2)/ perovskite(CH3NH3SnI3) / hole transport medium (CuI)/back contact as shown in Figure. 1.

Parameters for simulation of all layers are described in Table I

The research is based on observing the effects by adjusting the number of defects and the N_A of the perovskite layer of tin perovskite. No contacts resistance (Series/parallel) is taken here. Using flat bands the Work function of back contact has been calculated. Since of the self-doping phenomenon, the perovskite exhibits a conductive type of p-type, so it is in feed that the perovskite is p type semiconductor with primary doping concentration of 1.0×10^{15} cm^{-3}.

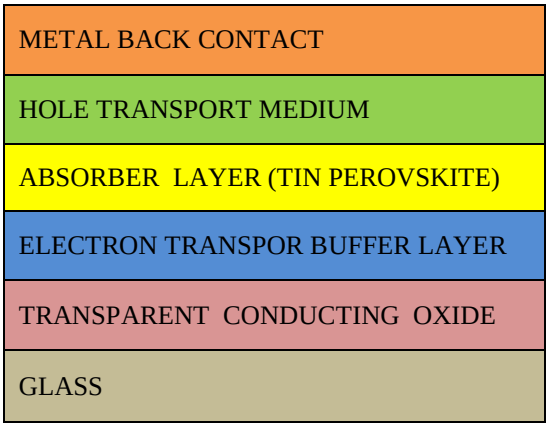

Fig. 1: Structure of the perovskite solar cell

Parameters	CO SnO_2:F	Buffer layer	Absorber layer ($CH_3NH_3SnI_3$)	HTL1spiro-OMeTAD	HTL 2 Copper Oxide(Cu_2O)[3]	HTL 3 Copper iodide(CuI)[14]
Thickness (nm)	500	50	350(variable)	350[15]	350	400
Band gap, E_g (eV)	3.5	3.25	1.3	3.17	2.1	3.1
Electron affinity (eV)	4	4.08	4.1	2.05	3.2	2.1
Relative Permitivity, ξ	9	9	8.2	3	7.11	6.5
Electron Mobility (cm^2/ Vs)	20	340-165	1.6	2×10^{-4}	3.4	44
Hole Mobility (cm^2/Vs)	10	50-5	1.6	2×10^{-4}	3.4	44
Concentration of donor impurity, N_D ($1/cm^3$)	2×10^{19}	10^{16}	-	-	-	-
Concentration of acceptor impurity, N_A ($1/cm^3$)	-	-	1.0×10^{15}	1×10^{18}	1×10^{18}	3×10^{18}
Defect Density, Nt	10^{15}	10^{18}	4.5×10^{17}	10^{15}	10^{15}	10^{15}

Table 1: Parameters for design simulation

III. Results and Discussion

The non-toxic tin based PSC is studied here using 1-dScaps simulation software.Fig.2 shows the simulated structure of perovskite solar cell. In the simulated structure the band diagram as shown in fig. 4 and other parameter can be easily calculated. The outcome shows that due to the enhanced built-in electrical potential, the adequate p-type carrier doping concentration of perovskite could improve device efficiency but overwhelming amount of concentration can contribute to higher recombination rates and degraded cell performance adjusting the buffer layer's electron affinity and HTM to provide a suitable interface obstacle for carriers can minimize the interface recombination and to some degree enhance device PCE. The defect density of the PSCs is the most important thing for the high efficiency of sun based cells. Reducing the concentration of density as low as 1×1015 cm-3 can remarkably enhance PCE from 6.09% to15.28%.

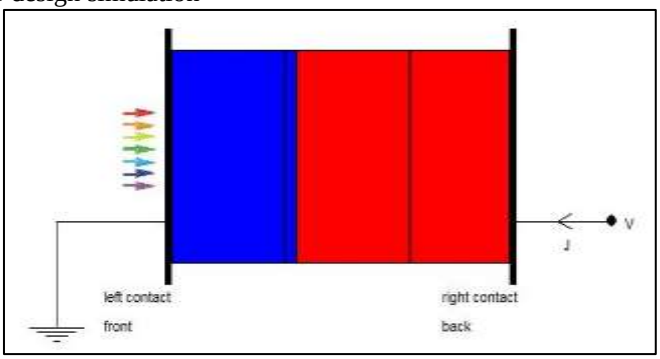

Fig. 2: Simulated design of perovskite solar cell

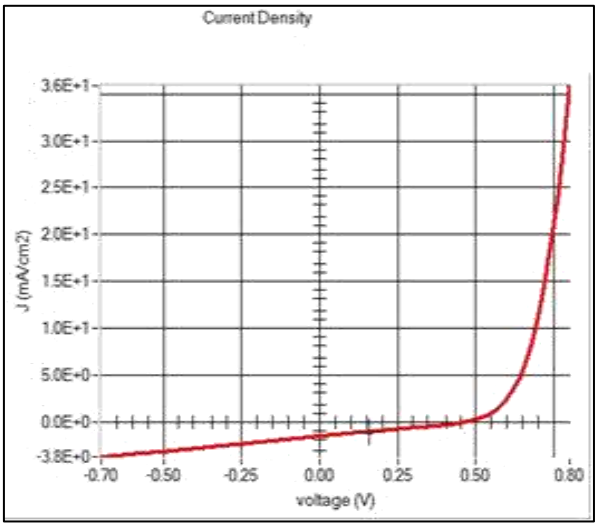

Fig. 3: J-V characteristics

The optimal thickness(perovskite) of 600 nm[16] can suck up by optimizing all of values. more light and improve the efficiency of the device to 16.50%. Uplifted results with PCE of 23.36% are acquired. In case of CuO_2 a better efficiency approx. 18% can be achieved in fact after optimization results can go up to 24%. After simulation with copper iodide as hole transport layer, by which results have been quite improved as compare to other materials. In the case of Copper iodide it can clearly analyze from the J-V curve fig.3 and quantum efficiency curve, fig. 5 the values for PCE, V_{oc}, J_{sc}, FF are 24.30, 0.917, 32.86, 80.60 % respectively. Therefore the results show that the $MASnI_3$ perovskites /CuI have the future to be highly productive PSCs [17] .

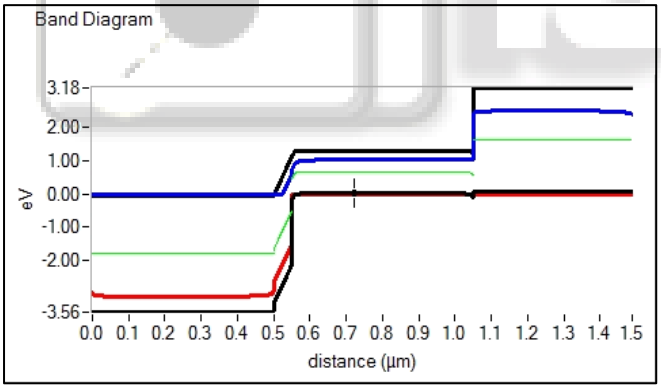

Fig. 4: Energy level diagram

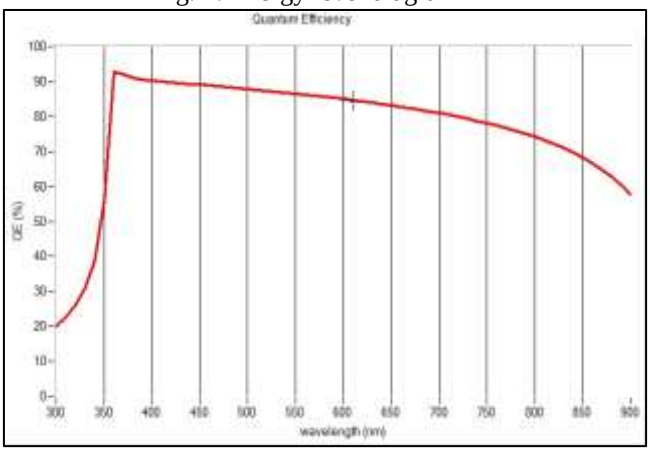

Fig. 5: Wavelength Vs. Quantum efficiency curve

By improving the stability of Sn^{2+} in $MASnI_3$ and reducing the defect density by optimizing the fabrication and encapsulation process, further efficiency of the lead free $MASnI_3$ perovskite solar cells can be increase.

IV. Conclusion

The device's performance parameters were carefully evaluated for the classification of critical specifications that define the overall conduct .In this research 1D device simulator is used to analyze and calculate different parameters of sun based non-toxic cell with spiro-OMeTAD, CuO_2 and CuI as HTM. Nt is the crucial parameter to be optimized to maintain the device's practicality. Doping profiles also have a dramatic impact on results. Default density is the crucial parameter that must be optimized to support the device's practicality. Although the trend of using lead free material is quite appreciable but indeed lot of work and research must be needed to do in the field of non- toxic perovskite solar cell to enhance the efficiency. There are some other factors also involve like stability issues and hysteresis effect which can be reduce by incorporation of device encapsulation.

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