PROSPECTS OF COPPER OXIDE AS A HOLE TRANSPORT MATERIAL FOR A HIGHLY EFFICIENT PEROVSKITE SOLAR CELL

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Abstract: Renewable sources are the ultimate solution to suffice the current energy crises present in the today's world. Dependencies on the energy requirements can't be snubbed in any case. Among the most worn renewable sources, Solar Energy is been the epitome of energy source. Solar cells, an idol of solar energy is the most preferred technology that is highly responsible for the fulfilment of energy needs. But an efficient source also requires a careful selection of the contributing attributes for its significant functioning. Among the main constituents, this paper mainly focusses on the prospects of inorganic material CuO (Copper Oxide) as a hole transport material. The result provides a clear indication of a highly efficient material and supports its use in the fabrication of perovskite solar cells. Simulation results concluded with an increase of 4.14% in power conversion efficiency, 4.05% increase in open circuit voltage and 2.621% enhanced short circuit current density.

***IndexTerms* - Perovskite solar cell, power conversion efficiency, solar cell, inorganic material**

I. INTRODUCTION

Contributing higher efficiencies, low manufacture costs, and huge optoelectronic properties, perovskites solar cells are the drifting point of research now a days. Because of the headways made in the ongoing years, it's additionally named as the quickest developing innovation which could contend the customary techniques for energy harvesting. This solar cell uses the perovskite compound as a functioning layer. The root of these solar cells lies under Dye Sensitized Solar Cells. The most normally utilized compound for such PV cell is natural inorganic lead or tin halide-based materials. This dynamic layer is in charge of the proficient light gathering in to the PV cells. Low manufacture cost and higher proficiency has made this innovation most encouraging till date. A colossal progression in the productivity of 22.1% from year 2003 to 2017 has been accomplished with this innovation, subsequently the quickest developing innovation. The fundamental concern or the disadvantage of this innovation is its reaction to the ecological factor. Natural variations like oxygen and dampness hamper the working of these PSCs which can be averted by advancing the constituting materials. The study is still on track to keep the debasement of these cells in the environmental conditions [1-5].

The active layer in the solar cell is the most imperative factor that administers the execution of the cell comprehensively. Methyl Ammonium Lead iodide is the generally used perovskite material for active/absorber layer because of its ample of optoelectronic properties [6]. The crystal structure has A and B are cations which lies in the corner of the unit cubic cell. X is the anion which is present at the face centre. Mixed halide perovskites yields significant optoelectronic properties [7] and has a high diffusion lengths > 1μm and furthermore confers high charge density and collection. A legitimate and an adjusted mix of electron transport materials (ETMs), active layer, and hole transport materials (HTMs) contributes towards the coveted yield comes about [8-12]. There are sufficient of choices accessible to be utilized as ETMs and HTMs however certain properties of these materials settle on them the best decision to be utilized as a part of creation. A careful decision with a basic learning and comprehension of material properties is a significant part in the creation procedure. There are wide scopes of natural and inorganic materials to be utilized as a HTM and ETM. Spiro-MeOTAD, PEDOT:PSS, P3HT, PTAA and so on are probably the most usually utilized natural HTMs [13-22]. These materials are expensive and somewhere lacks in chemical stability, durability, high manufacture cost and so on so the concentration is moved towards the inorganic HTM, for example, CuSCN, Cu2O, CuI and so on. Due to its captivating optoelectronic properties like stability, durability, and high absorption coefficients etc. these become potential candidates to participate in the device formation [23-24]. For ETMs, TiO2 and ZnO are most usually utilized semiconductor materials. Fitting bandgaps, electron mobility, and extensive surface region settle on them makes them a perfect choice to be utilized as ETM. Additionally these materials are copiously present on earth and give ease in creation forms. This investigation is fundamentally focussed on the traversing the potential of CuO as a HTM in the perovskite solar cell [25-26].

II. DESIGN SIMULATION METHODOLOGY

The basic structure simulated for the design of perovskite solar cell is TCO/ETM/IDL1/Absorber Layer/IDL2/HTM. Where IDL1 and IDL2 are the interfacial defect layers. These layers maintain the practicality of the device to make it comparable to the real time devices. Fig. 2.1 represents the basic device proposed for the efficient perovskite solar cell. The proposed design is simulated using SCAPS software and the potential of the constituting materials and its properties are analyzed. The software works basically

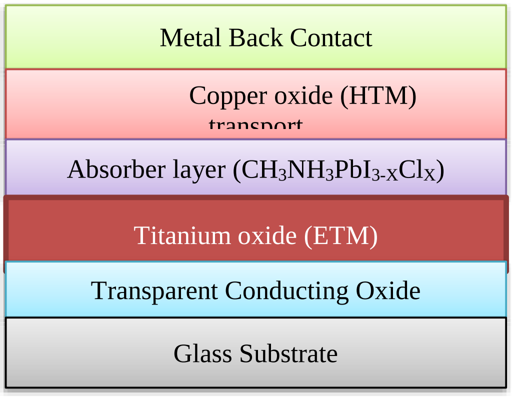

Fig. 2.1Layered architecture of Proposed Design

on the Poisson's equation and the continuity equations. The basic design parameters are considered for the device design is enlisted in Table 2.1. The above represented diagram is the resulting device structure after the optimization and simulating the proposed objectives of an efficient solar cell. The electron thermal velocity is taken1×107 cm/s for both the charge bearers. To fulfil the real time application, Gaussian defect density distribution is considered. Cross-section= 2×10 cm^{-2} is taken for both the charge transporters i.e. electrons and holes. The simulated design structure is represented in Fig. 2.2.

Table 2.1 Design Simulation Parameters

Parameters	TCO (SnO_2: F)	TiO_2	Defect Layer 1	Absorber Layer ($CH_3NH_3PbI_{3-X}Cl_X$)	Defect Layer 2	HTM (CuO)
Thickness(nm)	500	50	10	330	10	400
Band gap, Eg (eV)	3.5	3.2	1.55	1.55	1.55	3.1
Electron affinity,(eV)	4	3.9	3.9	3.9	3.9	2.1
Relative permittivity, ε	9	9	6.5	6.5	6.5	6.5
Effective conduction band density, N_C (cm^{-3})	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}	2.2×10^{18}
Effective valance band density, N_v (cm^{-3})	1.8×10^{18}	1.8×10^{18}	1.8×10^{18}	1.8×10^{18}	1.8×10^{18}	1.8×10^{18}
Electron/hole mobility, μ_{n}/μ_p ($cm^2V^{-1}s^{-1}$)	20/10	20/10	2/2	2/2	2/2	44 / 44
Donor/ Acceptor Concentration (cm^{-3})	2×10^{19}	1×10^{16}	10^{13}	10^{13}	10^{13}	3×10^{18}
Defect density, N_t (cm^{-3})	10^{15}	10^{15}	10^{10}	2.5×10^{13}	10^{10}	10^{15}

III. RESULT ANALYSIS AND DISCUSSION

The effect of various factors like the thickness, doping concentrations of the charge carries, defect densities, and also the interfacial defect densities is considered and analyzed in order to design an efficient solar cell.

3.1 Effect of thickness of ETM: The thickness of the contributing materials is an imperative part in choosing the characterizing parameter of a solar cell, as the generation and recombination are controlled by the thicknesses of the absorber layer and the constituting materials. The essential participating parameters are extricated from the Table 2.1.

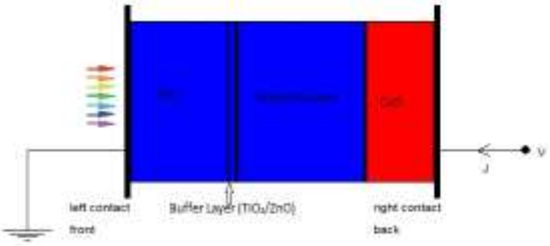

Fig. 2.2 Simulated Device Structure

The thickness of ETM layer is varied from 30nm -60nm. The champion device has PCE= 24.49%, V_{OC}= 1.16 4V, J_{SC}= 24.512 mA/cm^2, and FF= 86.13%. The device performs better under lower thickness of the ETM due to the partial absorption of charge carriers at the higher thickness as shown in Fig. 3.1. Also, the varying resistances with the increasing thickness also creates barrier in the higher charge generation.

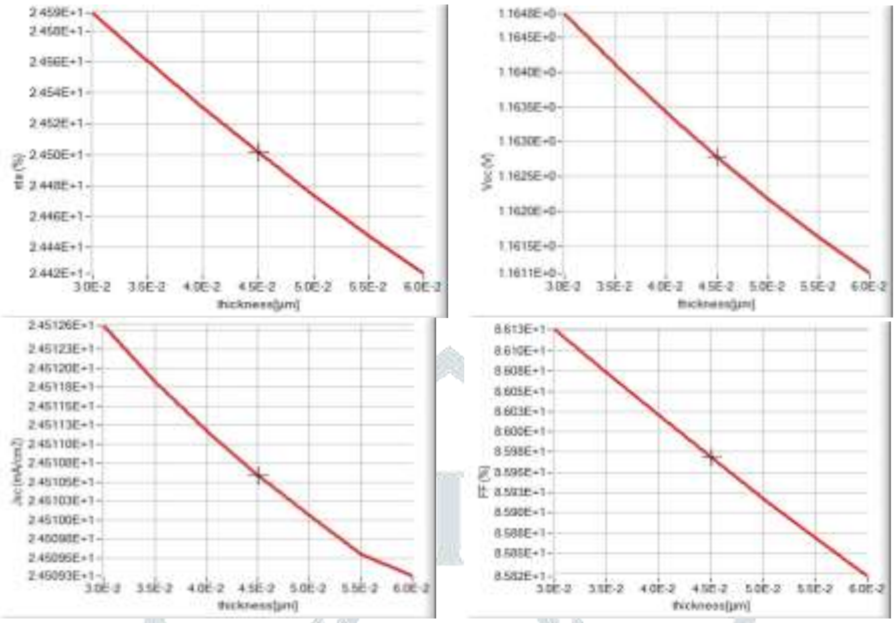

Fig. 3.1 Variation in cell parameters with the thickness of ETM

3.2 Thickness of Absorber Layer: The absorber layer's thickness is also a crucial parameter while defining the performance of any solar cell device. The absorber thickness directly deals with the generation and recombination of the charge carriers and hence directly affects the performance of the solar cell device. The mixed halide perovskite are most efficient in the range of 400 nm- 800nm. At the lower values of thickness of perovskite absorber layer, the efficiency count is least due to the improper absorption due to the smaller area. As the thickness expands, it prompts the yield voltage and fill factor diminishes as the thickness increments because of the increase in the present thickness and proficiency as can be clearly seen expansion in the no. of charge transporters and consequently from Fig. 3.2 resistance and recombination of the charge carriers. Solar cell of TiO_2 as ETM displayed greatest proficiency at 650 nm and began diminishing a short time later.

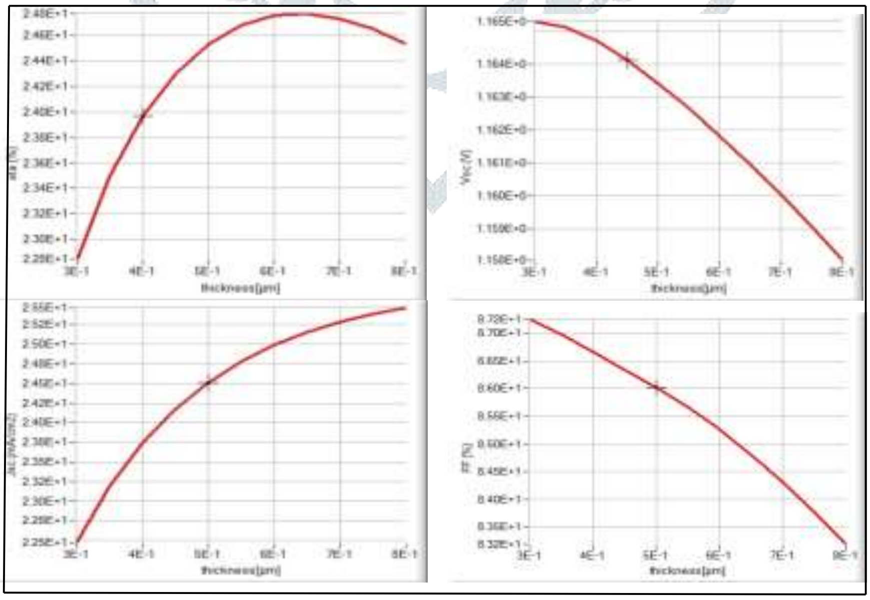

Fig. 3.2 Variation in cell parameters with a thickness of absorber layer

3.3 Doping Concentration of ETM: As in the ETMs, doping profile is an essential part to decide the execution of the solar cell. The ETM confer a similar conduct as in case of the variation in accordance with the absorber's thickness. The doping is changed from 1˟ 10^{15} cm^{-3}-1˟10^{21} cm^{-3} for both the device under consideration. The diagram in Fig.3.3 boosts for the higher qualities estimation of doping and expands at around 1.66˟ 10^{20} cm^{-3} and countenances degradation in a short time later because of the Moss Burstein Effect. Past this esteem, current thickness pointedly began diminishing because of lesser electron mobility. The highest obtained parameters values at this place are PCE=25.157 %, V_{OC}= 1.16 V, J_{SC}= 25.17 mA/cm^2, and FF= 85.62%.

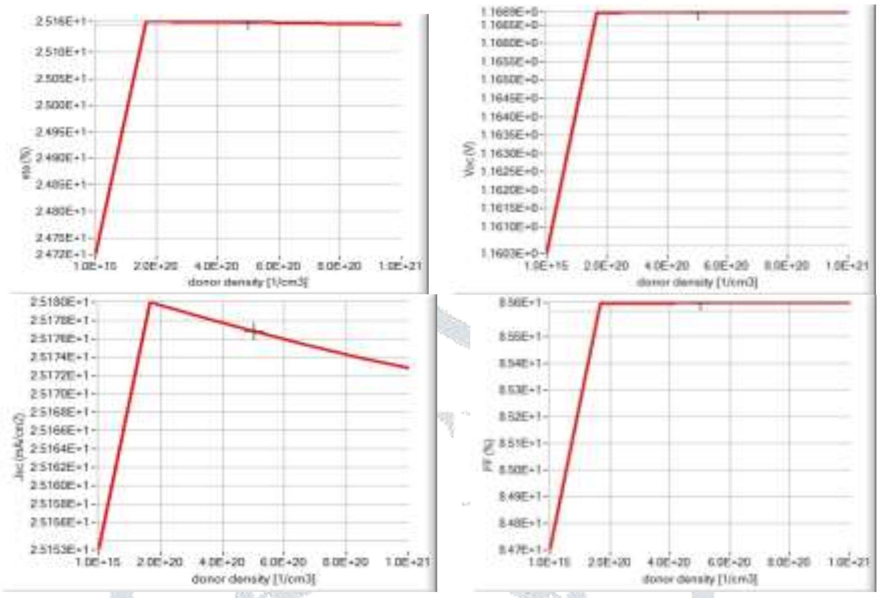

Fig. 3.3 Variation in cell parameters with a doping concentration of ETM

3.4 Defect Density: At first, the interface or the defect layers IDL1 and IDL2 between ETM/$CH_3NH_3PbI_{3-x}Cl_x$ and CuI/$CH_3NH_3PbI_{3-x}Cl_x$ separately are kept at defect level 1˟10^{15} cm^{-3} to keep up the real time influencing factors in solar cell devices. The charge carriers created at the active layer goes to the ETM and HTM and is highly affected by electric field through these interfaces. Thus these interfaces of the defect layers likewise require crucial choices. In the case of TiO_2/$CH_3NH_3PbI_{3-x}Cl_x$ interface layer, keeping defect thickness of active layer at 1˟10^{10} cm^{-3}, the PCE=26.42%, V_{OC}= 1.186 V, J_{SC}= 25.20 mA/cm^2, and FF= 88.38% are obtained as appeared in Fig. 3.4. As the imperfection expands, it causes the recombination of charge carriers before achieving the contacts of device materials because of uneven surfaces, henceforth hamper the performance. The solar cells with TiO_2 as electron transport material shows high performance at 1˟10^{13} cm^{-3} defect level of the defect layer at 1˟10^{13} cm^{-3} defect level of active layer. Accomplished PCE= 25.172%, V_{OC}= 1.167V, J_{SC}= 25.185 mA/cm^2, and FF= 85.64% is higher when contrasted with the outcome exhibited in [28].

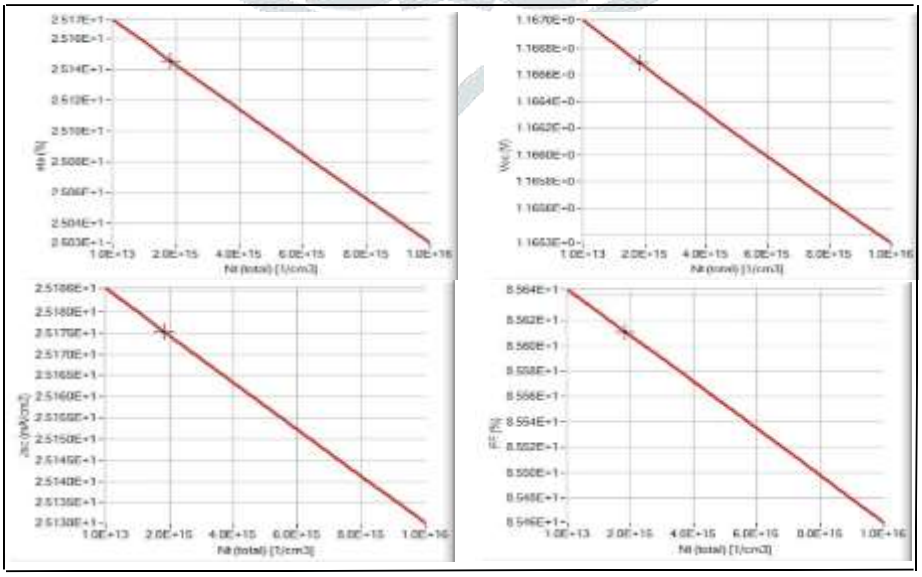

Fig.3.4 Variation in cell parameters with defect density in the interface layer with TiO_2

With the expansion in defects, the performance of the solar cell gets corrupted straight. The defect level at 1×10^{16} cm-3 drops the PCE to25.03%, V_{OC}= 1.165V, J_{SC}= 25.13 mA/cm^2, and FF= 85.46% as appeared in Fig. 3.4.

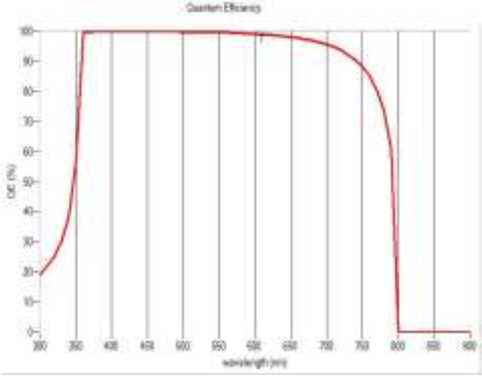

Fig. 3.5 Quantum efficiency Curve

The quantum efficiency curve for perovskite solar cell with CuO as HTM and TiO_2 as an ETM is represented in Fig.3.5. As can be clearly seen in the diagram, most extreme quantum effectiveness exists in the range of 300nm-800nm. The device moved toward greatest proficiency at right around 350 nm and stays consistent up to 600 nm range and covers a full unmistakable area of the range.

Table 3.1 Comparison between existing data and proposed design

Sr. No.	Parameters	Proposed Model	Model [27]	%age Improvement
1.	Power Conversion Efficiency (PCE), η, %	25.172	24.13	4.139%
2.	Open-Circuit Voltage (V_{OC}), V	1.167	1.12	4.051%
3.	Current Density (J_{SC}), mA/cm^2	25.18	24.52	2.621%
4.	Fill Factor (FF), %	85.64	87.75	-

Nonetheless, TiO2 some way or another keep up to exceed expectations the execution with bit higher powerful execution parameters. Table 2 gives information of the comparison of the proposed design with the existing device. The outcome demonstrates that a precisely upgraded and dissected perovskite solar cell with profoundly proficient TiO_2 as ETM and highly efficient CuO as an HTM performs superior to the current outcomes under similar conditions.

IV. CONCLUSION

A hypothetical report utilizing recreation program is done TiO_2 as ETM and CuO as an efficient HTM. An impact of parameters like thickness, doping concentration, and defect are majorly considered for the study. The result and analyses set future considerations for the inorganic HTM due to the effective conductivity, bandgap, high hole mobility and optoelectronic properties these offers. The result shows an increase of 4.14% in PCE, 4.051% in $V_{OC,}$ 2.621% enhanced $J_{SC.}$ The investigation uncovered that with an expansion in the thickness of the active layer, the PCE for the device increments. The solar cell device best performed at 650nm. The thickness of ETMs took after the contrary pattern, and execution diminishes with increment in the ETM thickness because of the partial absorption of the charge carriers' midway. High estimations of J_{SC}, V_{OC}, and FF point towards, high retention and low pinholes exhibit in the layers and subsequently the effective perovskite. The blended halide structure displayed a high diffusion length and added to higher PCE. The outcomes likewise demonstrate that the TiO2 needed some place in electron mobility and cost. The best-upgraded efficiencies achieved is 25.172% Careful manufacture process, a functioning active layer, highly mobile HTM and exceptionally specific contacts with very conductive ETM can balance out the gadget and enhance the performance too.

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