Journal of Current Research in Engineering and Science
Bi-Annual Online Journal (ISSN : 2581 - 611X)

Volume 6 –Issue 2,August 2023
Paper 53

Simulation of Metal oxide based thin film solarcell using Scaps 1D

G.Gokul Prasath
Electrical and Electronics Engineering
Sri Venkateswara College of Engineering
Sriperumbudur,Kanchipuram
gokulprasathg05@gmail.com

S.Akash
Electrical and Electronics Engineering
Sri Venkateswara College of Engineering
Sriperumbudur,Kanchipuram
akashsekar5445@gmail.com

KM.LathishKumar
Electrical and Electronics Engineering
Sri Venkateswara College of Engineering
Sriperumbudur,Kanchipuram
lathishkumar2000@gmail.com

S.Sinthamani M.E.,
Electrical and Electronics Engineering
Sri Venkateswara College of Engineering
Sriperumbudur,Kanchipuram
sinthamani@svce.ac.in

Dr. Sudhakar K Bharatan M.E., Ph.D,
Electrical and Electronics Engineering
Sri Venkateswara College of Engineering
Sriperumbudur,Kanchipuram
sudhakar@svce.ac.in

Abstract—***High-efficiency, low-cost thin film solar cells are an exciting option for generating cost-effective electricity through photovoltaic technology. Copper oxide thin films are particularly promising for use in thin film solar cells that can harness the visible and UV regions of the solar spectrum. Solar cells with efficiencies exceeding 30%, such as multi-junction III-V cells combined with silicon cells, are well-suited for automotive applications, where limited space on electric car rooftops is a key consideration.The researchers acknowledge, that these devices are still too costly and that further improvements in material and cell quality, as well as a reduction in resistance loss, should be achieved. In this work, we have optimized the CuO layer and implemented it in heterojunction solar cells as an absorption layer which gives an increase in efficiency due to the addition of ETL and HTL of layer. We have simulated the heterojunction solar cell using SCAPS 3.8. A solar cell can be described by the SCAPS as a series of layers with different optoelectrical properties, including the defect states of each layer and interface. We can simulate up to seven layers by considering the recombination mechanism, (band to band, Auger, SRH-type) and defects at interface level and bulk level. We have simulated a p-Cu0 with n-ZnOhetero junctionsolar cell inaddition to 10 nm thickness of MoS_2 as ETL and AZO as HTL layer giving the increase in efficiency of 26.04% from 24.15%.***

Keywords—CuO, ZnO, FTO, SCAPS, SRH,ETL,HTL

I. INTRODUCTION

The use of Photovoltaic technology allows for the direct conversion of abundant solar energy into electricity, thereby promoting environmental sustainability through the reduction of carbon emissions [8]. Copper oxides, including CuO and Cu2O, have shown potential as active absorber layers in photovoltaic devices [2]. These naturally occurring semiconductor materials are non-toxic, and their band gap energies range from 1.21 - 2.1 eV for CuO and 2.1 - 2.6 eV for Cu2O.

The absorber layer is a crucial component in achieving optimal PV performance, as it is responsible for the generation of photo excited charge carriers. The quality and morphology of the absorber layer directly impact the overall performance of the PV cell [11]. In this study, we utilized SCAPS ID to simulate a metal oxide thin film solar cell with CuO as the absorption layer [1]. SCAPS ID is a tool that describes a solar cell as a series of layers, including the defect states of each layer and interface. It is a versatile tool that can analyze homo and hetero junctions, multi junctions, and Schottky barrier photovoltaic devices [6]. All other simulation tools are for multi-stream applications but SCAPS 1D is specially designed for solar cell simulation alone, thus it yields more accurate results. It delivers an open source license and the interface is simple yet powerful. SCAPS 1D overcomes recombination analysis of solar model while other software lacks. Accounting all these parameters we have chosen SCAPS 1D as our base simulation software. Using this software we can simulate up to seven layers by considering the recombination mechanism, (band to band, Auger, SRH-type) and defects at the interface level and bulk level. In this work, we have simulated a CuO thin film with ZnO using Solar Cell Capacitance Simulator (SCAPS-1D) and studied the effect of absorption layer (CuO) thickness, defect density, and cell temperature on the performance of the cell. The effect of different electrodes gold, silver, molybdenum, copper (Au, Al, Mo, Cu) with ETL and HTL also have been studied [4].

II. METHODOLOGY AND SIMULATION PARAMETERS

Every photovoltaic device must obey:

$$\text{Conversion Efficiency } (\eta) \equiv \frac{\text{Output Energy}}{\text{Input Energy}}$$

For most solar cells, this breaks down into:

Journal of Current Research in Engineering and Science
Bi-Annual Online Journal (ISSN : 2581 - 611X)
Volume 6 –Issue 2,August 2023
Paper 45

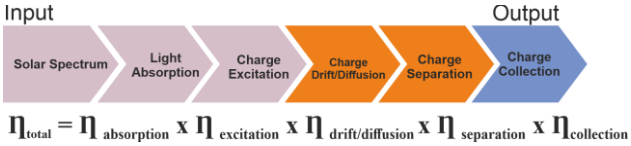

Fig. 1. Energy Conversion

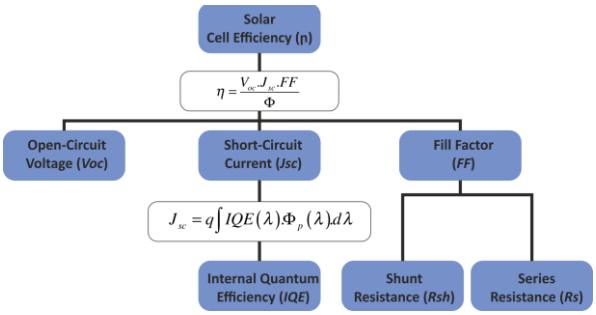

Fig. 2. Interrelation of solar cell efficiency with different parameters

Two engineering options are available when the material has a short minority carrier diffusion length relative to absorber thickness: reducing the absorber layer thickness or increasing the diffusion length. The current produced in an illuminated pn-junction device is limited by the minority carrier flux at the edge of the space-charge region.

$$J_{sc} \approx qGL_{diff} \quad (1)$$

$$J_{sc} \propto L_{diff} \quad (2)$$

$$Voc = \frac{k_B T}{q} \ln\left(\frac{J_{sc}}{J_o} + 1\right) \quad (3)$$

$$J_o \approx \frac{qDn_i^2}{L_{diff} N} \quad (4)$$

Where, J_{sc}=Illuminated current, G=Carrier generation rate, L_{diff}=Diffusion length

B. Device structure and simulation parameters 1

A. Effect of solar cell efficiency on different parameters

Efficient movement of photo-excited carriers is critical for the performance of a solar cell, as they must be able to travel from their point of generation to the collection point. Typically, longer diffusion lengths result in better PV performance, indicating that the carriers must be able to move a significant distance to be effectively collected.

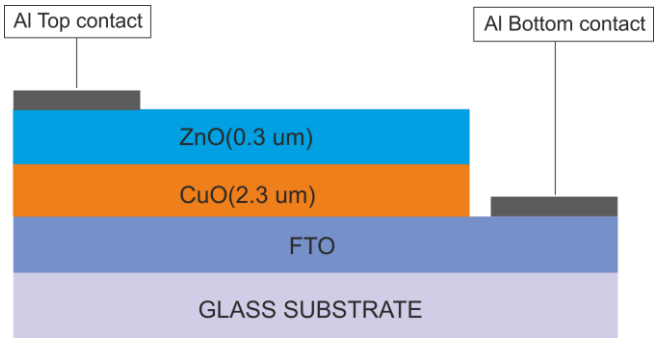

Fig. 3. Device Structure 1

Fig 3 shows the structure of a solar cell (FTO/CuO/ZnO/Al) with a thickness of 2.3µm for CuO and 0.3µm for n-ZnO on an FTO substrate, with aluminum used as contacts. Using SCAPS 1D, we simulated the same structure to optimize the thickness of the CuO layer, employing the simulation parameters shown in table I [3]. Among the three metals (Al, Mo, Cu) used as contacts, excluding gold (Au), all three yield an efficiency of approximately 22%. However, the efficiency of the solar cell with Au contact is 19%. Consequently, we conducted further analysis by incorporating a buffer layer of MoS_2 (Hole Transport Layer) and AZO (Electron Transport Layer) to evaluate the impact of defect density on the performance of the solar cell with the optimized CuO thickness of 2.3µm and aluminum as contacts.

TABLE I. Simulation Parameters

Properties	n-ZnO	p-CuO
Thickness (µm)	0.25	3.5
Band gap (eV)	3.3	1.6
Electron affinity (eV)	4.4	4.7
Permittivity	9	10.5
CB ($1/cm^3$)	2.20E+18	1.80E+19
VB ($1/cm^3$)	1.80E+19	4.00E+18
Electron mobility (cm^2/Vs)	5.00E+01	1.00E-01
Hole mobility (cm^2/Vs)	2.50E+01	2.50E+01
Electron thermal velocity (cm/s)	6.70E+07	1.10E+07
Hole thermal velocity (cm/s)	2.99E+07	4.16E+07

Journal of Current Research in Engineering and Science
Bi-Annual Online Journal (ISSN : 2581 - 611X)
Volume 6 –Issue 2,August 2023
Paper 45

N_D (1/cm^3)	1.00E+18	0.00E+00
N_A(1/cm^3)	0.00E+00	1.00E+14

C. Device structure and simulation parameters 2

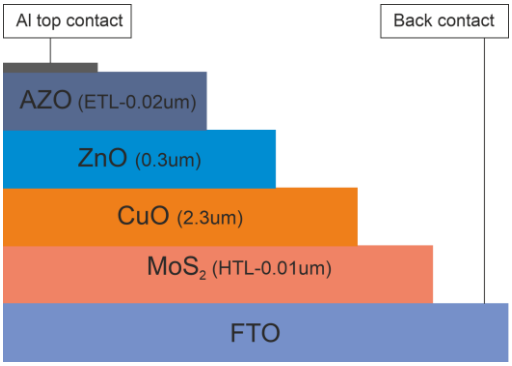

Fig. 4. Device Structure 2

Fig 4 displays the structure (FTO/MoS_2/CuO/ZnO/AZO/Al) of a solar cell featuring an additional Hole Transport Layer (MoS_2) and Electron Transport Layer (AZO) aimed at enhancing the efficiency of the proposed solar cell [15] [14]. The incorporation of a Hole Transport Layer facilitates the movement of positively charged holes from the active layer to the electrode [12]. Similarly, the Electron Transport Layer aids in the transportation of negatively charged electrons from the active layer to the cathode. We simulated optimized thicknesses of 0.01µm and 0.02µm for HTL and ETL, respectively. The inclusion of HTL and ETL is crucial in solar cell simulation as they optimize charge carrier transport and minimize recombination losses, thereby improving device efficiency and performance.

Also the interfacing layers is essential for minimizing energy barriers, enhancing charge extraction and maximizing the overall device performance.

III. RESULTS AND DISCUSSION

A. Effect of absorber thickness on the performance of the solar cells

To investigate the influence of the absorber's thickness, the simulation was carried out by keeping all other device parameters constant, ranging the thickness from 0.1 µm to 4 µm. The thickness of the active layer is a critical parameter that must be chosen meticulously to maximize current density while simultaneously minimizing the reverse saturation current [2].

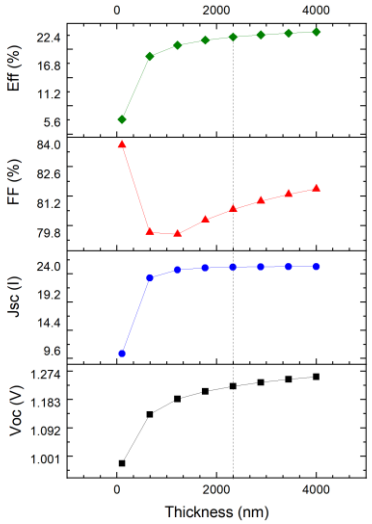

Fig. 5. Effect of absorber thickness on the performance of the solar cell

Fig 4 demonstrates the impact of absorption layer thickness on Voc, Jsc, FF and efficiency in solar cells. It is crucial to optimize the thickness of the absorbing layer in order to achieve desired performance. A too small thickness results in lower photocurrent, while an excessively thick absorbing layer leads to increased series resistance, material consumption, and overall cost per unit of power produced [9]. In the case of the depicted graph.Voc and Jsc show an increasing trend from 0.3µm to 2.3µm, but beyond this value, they start to decrease. Notably, at 2.3µm thickness, the efficiency reaches 22.84% with aluminum contacts.

B. Effect of defect density on the performance of the solar cells

Defects reduce solar cell efficiency by providing new recombination pathways (loss), by allowing the light to generate heat rather than electricity. Defects induce deep energy levels in the semiconductor bandgap, which degrade the carrier lifetime and quantum efficiency of solar cells. One of the most reasons is the existence of recombination centers, which trap photo generated carriers before they reach the solar cell terminals. Defects introduce energy levels in the bandgap, and act as recombination centers, which reduce the free carrier lifetime [7].

Journal of Current Research in Engineering and Science
Bi-Annual Online Journal (ISSN : 2581 - 611X)
Volume 6 –Issue 2,August 2023
Paper 45

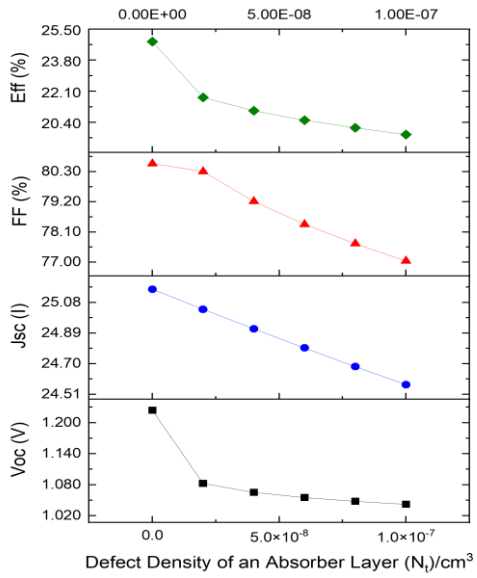

Fig. 6. Effect on defect density of anCuO on the performance of the Solar cell

Considering the defects level in the range of 10-7 to 10-9 with radiative recombination, Fig 5 illustrates the simulated graph depicting the relationship between defect density and various solar cell parameters such as Voc, Jsc, FF, and Efficiency. The achieved efficiency in this simulation is 24.64% [11] [12].

C. Effect of ETLand HTLon the perfomance of the solar cell

Electron transport layer using different materials such as Tin oxide (SnO_2), Tungsten tri oxide (WO3), Aluminum doped Zinc oxide (AZO) is simulated with existing device structure out of which Aluminum doped Zinc oxide (AZO)

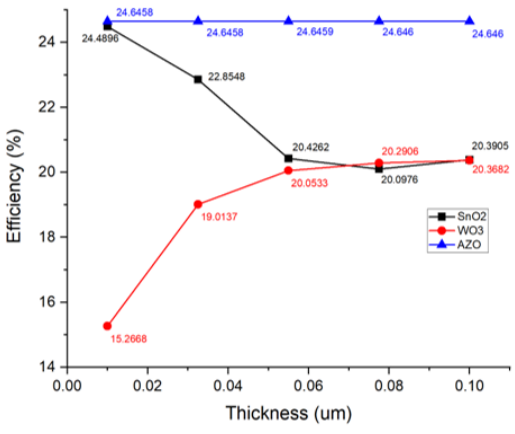

Fig. 7. Effect of ETL on the performance of the device

gives better results. The hole transport layer with different materials such as Molybdenum disulfide (MoS_2), Copper Indium (CI) and Molybdenum trioxide (MoO_3) and with range of thickness from 10nm to 100nm were simulated with existing device structure, The results shows (Fig 8) that the material Molybdenum disulfide (MoS_2) with10nm yields better efficiency of 26.04% which is greater than reported earlier [3]

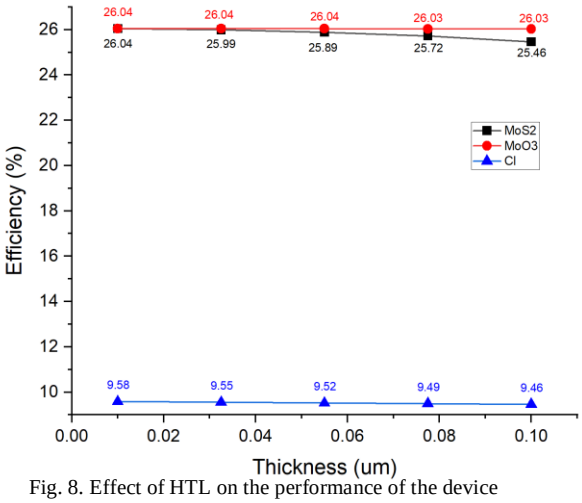

Fig. 8. Effect of HTL on the performance of the device

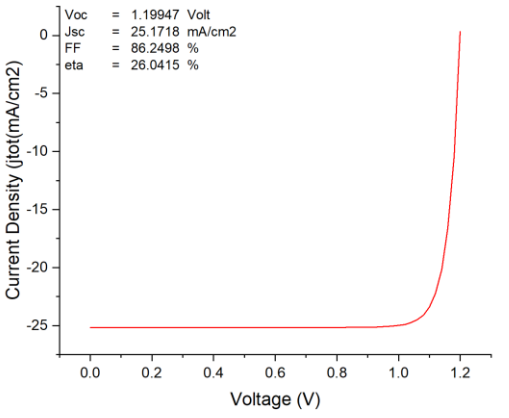

Fig. 9. Effect of HTL and ETL on the performance of the device

Journal of Current Research in Engineering and Science
Bi-Annual Online Journal (ISSN : 2581 - 611X)
Volume 6 –Issue 2,August 2023
Paper 45

IV. RESULT SUMMARY

SI No	Device Structure	Voc (V)	Jsc (mA/cm^2)	FF (%)	Efficiency (%)
1.	FTO/CuO/ZnO/Al	1.22	25.16	80.56	24.84
2.	FTO/CuO/ZnO/Mo	1.22	24.93	75.12	22.88
3.	FTO/CuO/ZnO/\Cu	1.22	24.96	80.54	24.63
4.	FTO/CuO/ZnO/Au	1.12	24.93	69.51	19.45
5.	FTO/CuO/ZnO/Al (With Recombination)	1.19	25.16	82.11	24.64
7.	FTO/MoS_2/ CuO/ZnO/AZO/Al	1.19	25.17	86.24	26.04

TABLE II. Results

V. CONCLUSION

In this study, we have simulated a heterojunction solar cell with the structure of FTO/MoS_2/CuO/ZnO/AZO/Al using SCAPS-1D simulation package. In our study, we conducted simulations and analyzed the impact of varying thicknesses of CuO absorption layer (ranging from 10 nm to 3 µm), defect density, and cell temperature on the performance of the photovoltaic device. The device shows the efficiency of 24.04% (without the ETL and HTL layer) absorption layer thickness of 2.3µm with aluminum as top and bottom electrode. The effect of electrodes has also been studied with four metal contacts like Au, Al, Mo, Cu out of these except Au other three metal yield the efficiency of 24% . Based on the cost of material we choose Aluminum as contact which will be suitable for large scale production. Simulated results as efficiency of solar cell with different metal electrodes, materials for ETL and HTL layers.
.

VI. REFERENCE

[1] Marc Burgelman, Koen Decock, Alex Niemegeers, Johan Verschraegen, and Stefaan Degrave, "SCAPS manual," December 2021.

[2] Adil Sunny, and Sheikh AI Ahmed , " Numerical simulation and performance evaluation of highly efficient Sb_2,Se_3 solar cell with Tin Sulfide as hole transport layer," physica status solidi (b) 258(7), April 2021.

[3] Abdul Kuddus, Md.Ferdous Rahman, S.Tabassum, J.Hossain, and Adu Bakar Md.Ismail, "Study on the performance of ZNO/CUO heterojunction solar cell,"International Conference on Computer, Communication, Chemical, Materials and Electronic Engineering (IC4ME2), July 2019.

[4] Numeshwar Kumar Sinha, Priyanka Roy, Dhriti Sundar Ghosh and Ayush Khare, "Simulation and analysis of schottky junction perovskite solar cells(SJPSES)," IOP Conference Series Materials Science and Engineering 1120(1):012017, December 2021.

[5] Paul A.Anderson, "The work function of copper,"British Journal of Applied Physics 15(8):94, April 1949

[6] Sonia Rani, Diganta Kuar, Vignesh Jeyachandran and Dhriti Sundar Ghosh, "Optoelectrical modeling of CsPbBr3 based all inorganic perovskite solar cell," Optical Materials, 2022, p. 112612, September 2022.

[7] Salvador Dueñas, E. Pérez, H. Castán, H. García, and L. Bailón, "The role of defects in solar cells: Control and detection," Electron Devices (CDE), 2013 Spanish Conference, May 2013.

[8] S.Sinthamani, M.Ranjithkumar, S.Anitha, S.Sudharsanam, M.Sasikala and Sudhakar K Bharatan, "Optical characterization of RF sputtered copper oxide for thin film solar cell application," Materials Today, January 2022.

[9] M.M Isa, Ibrahim Mustapha and A.A Yahaya. "Numerical Modelling Of The Effect Of Temperature And Thickness On The Electrical Properties Of Polycrystalline Semi-ConductorSolar Cells [CdTe and Cu(In, Ga)Se (CIGS)]Using One Dimensional Device Simulation," IOP Conference Series Earth and Environmental Science 730(1):012027, September 2021.

[10] Most. Marzia Khatun, Adil Sunny and Sheikh Rashel Al Ahmed. "Numerical investigation on performance improvement of WS2 thin-film solar cell with copper iodide as the hole transport layer,"Solar Energy Volume 224, Pages 956-965, August 2021.

[11] Priyanka Roy, Numeshwar Kumar Sinha, Sanjay Tiwari, and Ayush Khare, ". Influence of defect density and layer thickness of absorption layer on the performance of tin based perovskite solar cell,"IOP Conference Series Materials Science and Engineering 798(1), December 2019.

[12] Touria Ouslimane, LHoussayne Et-taya, Lahoucine Elmaimouni, and AbdellahBenami, "Impact of absorber layer thickness, defect density, and operating temperature on the performance of MAPbI3 solar cells based on ZnO electron transporting material," Heliyon. 2021 Mar; 7(3): e06379.

[13] Yi-Chun Chin, Matyas Daboczi, Charlie Henderson, Joel Luke, and Ji-Seon Kim, "Suppressing PEDOT: PSS Doping-Induced Interfacial Recombination Loss in Perovskite Solar Cells,"ACS Energy Letters 7(2):560-568, Jan 2022.

[14] Manas Tripathi, Vipul Vaibhav Mishra, Brajendra S. Sengar and A.V. Ullas, "Lead-free perovskite solar cell by using SCAPS-1D: Design and simulation",Optik - International Journal for Light and Electron Optics 229(10):166258, April 2022.

[15] Atanu Baga, R. Radhakrishnan, Reza Nekoveic, and R. Jeyakumard, "Effect of absorber layer, hole transport layer thicknesses, and its doping density on the performance of perovskite solar cells by device simulation," Solar Energy, vol. 196, pp. 177-182,January 2020.

[16] Laura Calil, Samrana Kazim, Michael Gr-tzel, and Shahzada Ahmad, "Hole-Transport Materials for Perovskite Solar Cells," Angewandte Chemie International Edition 55(47), October 2016

Faiza Azri, Afak Meftah, Nouredine Sengouga, and Amjad Meftah, "Electron and hole transport layers optimization by numerical simulation of a perovskite solar cell," Solar Energy 181, February 2019.

Journal of Current Research in Engineering and Science
Bi-Annual Online Journal (ISSN : 2581 - 611X)
Volume 6 –Issue 2,August 2023
Paper 45