Enhancement of performance of TiO_2/Cu_2O solar cells

B. ZAIDI[1,*], A. KERBOUB[1], T. BOUARROUDJ[2], C. SHEKHAR[3], T. MAHMOOD[4], M. A. SAEED[5]
[1]*Department of Physics, Faculty of Material Sciences, University of Batna 1, Batna, Algeria*
[2]*Scientific and technical research center in physico-chemical analyses (CRAPC), BP 384, Bou-ismail, RP 42004, Tipaza, Algeria*
[3]*Department of Applied Physics, Amity University Gurgaon, Haryana, 122413, India*
[4]*Department of Physics, GCW University, Sialkot, Pakistan*
[5]*Department of Physics, Division of S&T, University of Education, Lahore-Pakistan*

The TiO_2/Cu_2O heterojunction solar cell was investigated in the study given by using the Solar Cell Capacitance Simulator (SCAPS). It has been thoroughly investigated how different layer factors, such as thickness, defect density and acceptor density affect cell performance. The efficiencies (η) of solar cell were shown to be influenced by the thickness of the absorber (Cu_2O) and buffer (TiO_2) layers using numerical analysis. TiO_2/Cu_2O optimized solar cell design demonstrated potential efficiency of about 23%. We then looked at how temperature affected the photovoltaic efficiency.

(Received June 10, 2023; accepted November 24, 2023)

Keywords: Absorber layer, Electron transport layer, Solar Cell,TiO_2, Cu_2O

1. Introduction

The most encouraging semiconductors for the photovoltaic (PV) applications are the metal oxide semiconductors (MO). Because many MOs are non-toxic, chemically stable, and rich which permits material deposition under surrounding conditions [1]. MOs are already widely used in a variety of current commercial applications as active or passive components, such as the active channel layer in the transistors that make up the active matrix of displays [2] or the transparent conducting front electrodes and electron or hole transport layers in solar cells [3]. Due to its potential to lower costs by utilizing inexpensive materials and production techniques, heterojunctions fully based on MOs, also known as all-oxide photovoltaic cells, have recently attracted a great deal of attention [4-6].

TiO_2 is a well-known photo-catalytic material and an n-type semiconductor with a wide band-gap energy of 3.2 eV [7]. A dye-sensitized solar cell (DSSC), also known as a Grätzel cell, was created by Grätzel et al. and can increase efficiency by 11% when ruthenium dye is used [8]. However, there are issues with dye desorption, leakage, packing, and long-term stability with the Grätzel cell. The cells have undergone a number of improvements. One possibility is to change the cell from a liquid electrolyte to a solid-state cell by employing a p-type semiconductor as a hole conductor. In an effort to convert cells into solid-state DSSCs, a range of p-type semiconducting materials, including Spiro-OMeTAD [9] and copper (I) iodide (CuI) [10-11], have recently been used. However, interaction between the dye monolayer and the p-type material is crucial in solid-state DSSCs. Previous attempts to address these difficulties have failed since only partial filling of the TiO_2 pores with a p-type material was achieved, especially when thicker films were used.

One way to overcome the problems with solid-state DSSCs is to use ETA (extremely thin absorber) solar cells or quantum dot (QD) sensitized solar cells, which are conceptually similar to solid-state DSSCs [12–15]. In those solar cells, a small band-gap p-type semiconductor, such as $CuInS_2$, CdTe and SnS replaces the molecular dye in the DSSC and works as a photon absorber in the cells [16–18]. The semiconductor typically covers the n-type semiconductor film, which is usually TiO_2. The structure of the ETA and QD solar cells has the advantage of enhanced light harvesting due to surface enlargement and multiple scattering [7,8]. The TiO_2/CdTe cells fabricated by Ernst et al. [16] exhibited an open-circuit voltage of 0.67 V and a short-circuit current of 8.9 mA/cm^{-2} under 100 mW/cm^{-2} of simulated sunlight. Nanu et al. [17] generated $TiO_2/CuInS_2$ solar cells using an atomic layer chemical vapor deposition method (ALCVD) with 4% solar energy efficiency.

The most well studied system is heterojunction ZnO/Cu_2O cells [19], where the wide bandgap ZnO serves as a window layer and the Cu_2O has a bandgap at around 2 eV in the visible spectrum of the sun [20]. The impressive light to electric power conversion efficiencies have been recorded for cells with a ZnO window layer up to 4%, [21] while 5% were attained with a Ga_2O_3 layer [22], despite the Cu_2O bandgap not being appropriate for sunlight (AM1.5G). Recently, a Ga_2O_3/Cu_2O heterojunction cell was reported to have an open circuit voltage of up to 1.2 V [23]. The Cu_2O bandgap is virtually optimal for multi-junction tandem cells with three or more connections [24]. Cu_2O is also a very desirable absorber for semi-transparent photovoltaics. Cu_2O thin films have been used in optoelectronic devices such thin film transistors in addition to solar cells [25].

Solar Cell Capacitance Program (SCAPS-1D) numerical simulations of solar cells have been reported. Planar thin-film CdS/CdTe solar cells and CdS/CdTe nanowires were simulated by Anwar et al. [26]. They showed that the CdS nanowires increase the CdS/CdTe solar cells' efficiency by about 3%. It has also been examined how temperature, interface state density, and

interface surface recombination velocity affect CdS/CdTe nanowire solar cells. For thin film solar cells, Decock et al. [27] simulated multivalent defects with up to five different charge states and examined the properties of current density-voltage (J-V) and capacitance-frequency (C-f). They came to the conclusion that flaws affect the simulation's outcomes [27]. For polycrystalline CdTe and CuInSe films, Niemegeers et al. [28] created a numerical simulation device to determine the J-V and C-f properties. Then, comparisons between numerical simulations and actual measurements were made. For a trustworthy interpretation of doping profile measurements, numerical simulations can be utilized. The concordance between simulations and measurements was examined by Burgelman et al. [29] who modelled CdTe and Cu(In, Ga)Se_2 solar cells and presented the outcomes of J-V, capacitance-voltage (C-V), and C-f simulations. n-TiO_2/p-CuO and n-TiO_2/p-Cu_2O heterojunction solar cells were simulated by Sawicka-Chudy et al. [30] who also examined the impact of layer thickness and defect density in buffer and absorber thin films on cell performance. On the basis of the numerical simulations, Sawicka-Chudy et al. [31] also provided numerical research of J-Vcurves for n-TiO_2/p-Cu_2O solar cells and confirmed the potential usage of the n-TiO_2/p-Cu_2Ostructure.

However, there are still problems that need to be solved, such as the optimum work configuration, ideal material qualities, desired, and boundary work conditions for high cell performance. As a result, the authors made the decision to continue their research on structural analysis in order to obtain thorough results.

2. Methods

The schematic diagram of the proposed device is shown in (Fig. 1). The solar cell structure consists of three different layers: TiO_2 (buffer), Cu_2O monolayer (absorber) and the substrate. The proposed structure was simulated with the help of SCAPS-1D. The carrier transport and recombination process at the interface was investigated using Shockley-Read-Hall (SRH) interface approach.

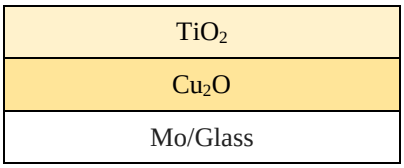

Fig. 1. Structure of the solar cell simulated by using SCAPS-1D

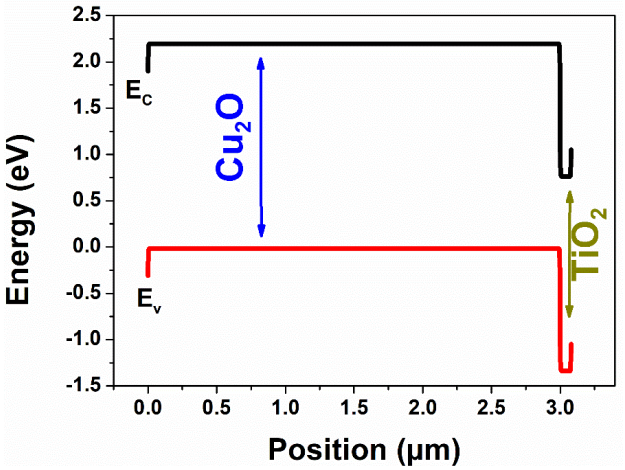

Fig. 2. Band gap diagram

Fig. 2 describes the energy diagram for the proposed structure of solar cell. It infers the electron affinity and band gap of the simulated solar cell. The obtained bandgap values of Cu_2O and TiO_2 are 2.15 eV respectively which are in the range. The band gap diagram was drawn using parameters as: solar spectrum AM1.5, P = 100 mW/cm^2, and T = 300 K. Other basic numerical parameters used in simulation of proposed solar cell layers are given in (Table 1).

Table 1. Materials and interface Parameters used in SCAPS-1D simulation

Parameters	**n-TiO_2**	**p-Cu_2O**
Eg (eV)	2.26	2.17
Electron affinity (eV)	4.2	3.2
Dielectric permittivity	10	7.11
CB effective density of states (cm^{-3})	2.2 x 10^{18}	2.2 x 10^{18}
CB effective density of states (cm^{-3})	1.8 x 10^{19}	1.8 x 10^{19}
μ_n (cm^2/V.s)	100	200
μ_p (cm^2/V.s)	25	80
Parameters (Unit)	**TiO_2/Cu_2O interface**	
Type of defect	Neutral	
Electrons capture cross-section (cm^{-2})	1 x 10^{19}	
Holes capture cross-section (cm^{-2})	1 x 10^{19}	
Reference for defect energy level (eV)	Above the highest eV	
Energy with respect to reference (eV)	0.6	
Total defect density (cm^{-2})	1 x 10^{11}	

3. Results and discussion

3.1. Effect of thickness

The solar cell's most crucial component is the absorber layer, which is where incident photons are absorbed, and excess carriers are produced. The n-buffer layer's primary

function is to join the p-absorber layer at a p-n junction. To reduce the PV device's series resistance, the buffer layer should be as thin as possible [30].

By varying the thickness from 1.0 to 9.0 nm (Cu_2O) and from 0.02 to 0.08 nm (TiO_2) without introducing additional defects, the effect of absorber and buffer layer thickness on cell efficiency (η) is simulated in this study (Figs. 3, 4).

Cell efficiency decreases linearly in relation to TiO_2 layer thickness in the TiO_2/Cu_2O structure. As a result, the TiO_2 buffer layer's optimal thickness for the current study has been set at 0.08 nm for TiO_2/Cu_2O . This indicates a cell efficiency of 22.65 percent.

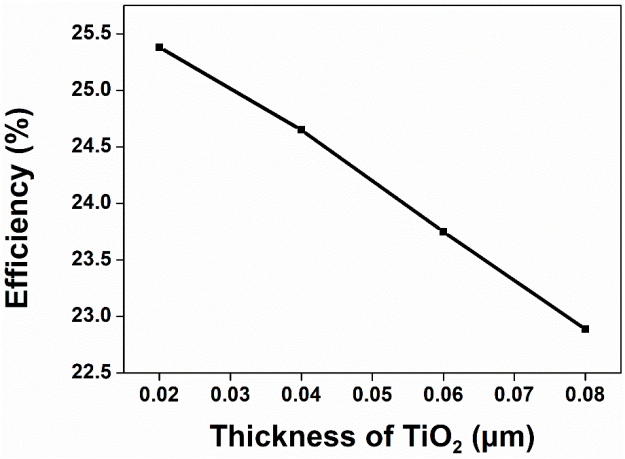

Fig. 3. Thickness of TiO_2 layer effect on the efficiency

It is essential to note that the curves in Figs. 3 and 4 have distinct trends. As the thickness of the Cu_2O layers increases, the efficiency of the solar cell initially increases and eventually reaches saturation at higher values. Nonetheless, as the thickness of the TiO_2 layers increases, so does the efficiency of the solar cell. The layers of Cu_2O can take in more photons and generate more current as the layer's thickness increases, which are mostly due to the thicker absorber layer's increased ability to absorb incident light [31]. Due to the limited diffusion length of the carrier, an increase in absorber thickness increases the likelihood of SRH (Shockley-Read-Hall) recombination, which results in this efficiency. As a result, the optimal thickness for the Cu_2O absorber was set at 3.0 nm for the current investigation. The cell is 22.65 percent efficient.

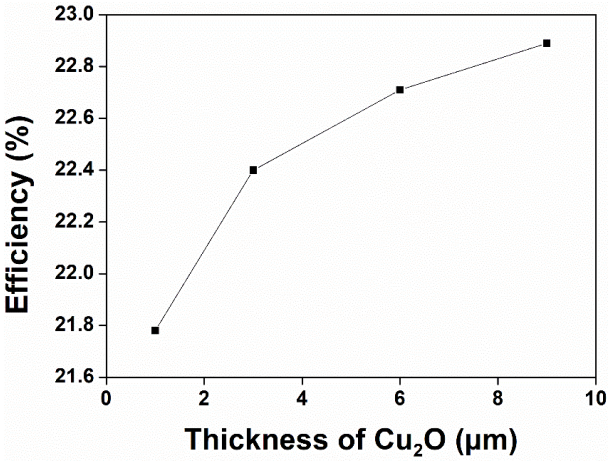

Fig. 4. Thickness of Cu_2O layer effect on the efficiency

3.2. Effect of defect density in n-TiO_2 and acceptor density in p-Cu_2O

The efficiency of proposed solar cell was also investigated in context of natural defects density in n-TiO_2 buffer layer. (Fig. 5) shows the variation in efficiency for density in the range from 10^{17} to 10^{20} cm^{-3}, however the thickness of n-TiO_2 buffer layer was kept as 50 nm. The observed improvement in efficiency can be justified by the introduction of additional carrier recombination centers within the layer [32].

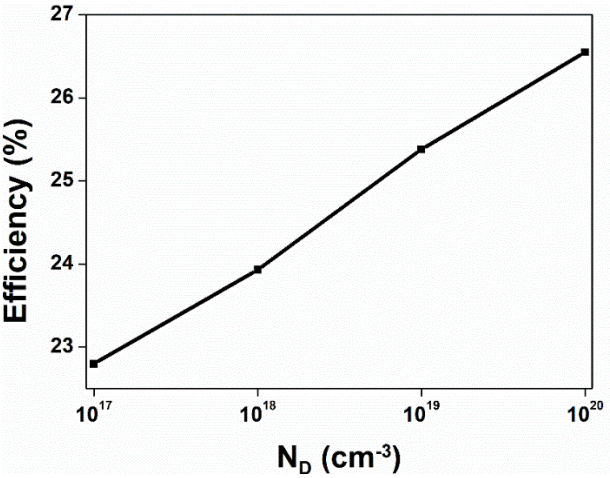

Fig. 5. N_D of TiO_2 layer effect on the efficiency

The efficiency of Cu_2O based solar cell was observed to increase from 24.6 to 25.7 % as the Cu_2O acceptor density varies from 10^{17} to 10^{20} cm^{-3} leading to the availability of added charge carriers for conduction within the cell as shown in (Fig. 6).

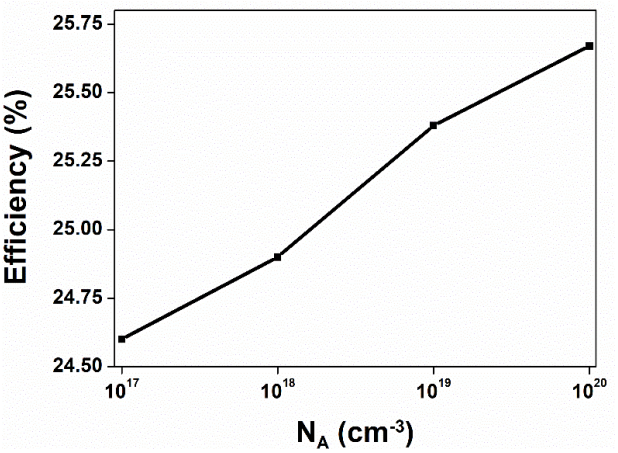

Fig. 6. N_A of Cu_2O layer effect on the efficiency

3.3. Effect of temperature on efficiency

The temperature plays a significant role in achieving the highest efficiencies of the solar cell. The temperature range is varied from 0°C-40°C. It can be inferred from the (Fig. 7) that with increase in temperature, the efficiencies of the solar cells decrease. This is due to increased recombination rates due to increased carrier concentration [33].

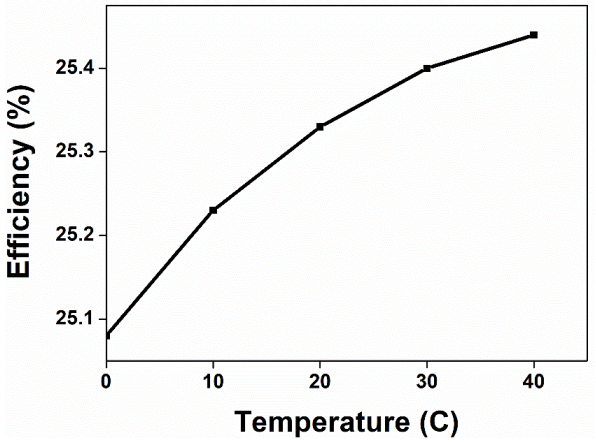

Fig. 7. Temperature effect on the efficiency

4. Conclusion

Using the SCAPS-1D solar cell simulator, the TiO_2/Cu_2O structure was examined in this work. A sophisticated simulation model of TiO_2/Cu_2O structure was finished by the analysis of the literature. Different parameters, including thickness (Cu_2O and TiO_2), defect density, acceptor density and temperature were tuned for the solar cells.

We have shown, via modelling, that changes in the absorber layer's thickness have a significant impact on conversion efficiency. The optimal value of the cell thickness was found to be 3.0 nm for the Cu_2O and 0.03 nm for the TiO_2 layer after the photovoltaic parameters were calculated.

We can also state that the defect density has a substantial effect on the performance of TiO_2/Cu_2O solar cell. With efficiency of 22.65% for the TiO_2/Cu_2O structure it demonstrated the high potential for proposed structure optimization. The technology trials that result in the development of the optimization cell will use the acquired information in practice.

Acknowledgements

The authors would like to express their sincere gratitude to Marc Burgelman and his team at The University of Ghent for providing access of SCAPS-1D.

References

[1] R. Jose, T. Velmurugan, R. Seeram, J. Am. Ceramic. Soc. **92**, 289 (2009).
[2] E. Fortunato, P. Barquinha, R. Martins, Adv. Mater. **24**, 2945 (2012).
[3] B. Zaidi, M. S. Ullah, B. Hadjoudja, S. Gagui, N. Houaidji, B. Chouial, C. Shekhar, Journal of Nano and Electronic Physics **11**, 02030 (2019).
[4] E. Fortunato, D. Ginley, H. Hosono, D. C. Paine, MRS Bull. **32**, 242 (2007).
[5] S. Rühle, A. Y. Anderson, H. N. Barad, B. Kupfer, Y. Bouhadana, E. Rosh-Hodesh, Arie Zaban, J. Phys. Chem. Lett. **3**, 3755 (2012).
[6] H. Bitam, B. Zaidi, B. Hadjoudja, C. Shekhar, S. Gagui, M. S. Ullah, Applied Solar Energy **58**, 198 (2022).
[7] J. Morasch, S. Li, J. Brötz, W. Jaegermann, A. Klein, Phys. Status Solidi A **211**, 93 (2014).
[8] A. Fujishima, K. Honda, Nature **238**, 37 (1972).
[9] M. Grätzel, J. Photochem. Photobiol. C **4**, 145 (2003).
[10] B. Zaidi, M. Zouagri, S. Merad, C. Shekhar, B. Hadjoudja, B. Chouial, Acta Physica Polonica A **136**, 988 (2019).
[11] K. Tennakone, G. R. R. Kumara, A. R. Kumar-Singh, K. G. U. Wijayantha, P. M. Sirimanne, Semicond. Sci. Technol. **10**, 1689 (1995).
[12] A. Atli, A. Yildiz, Appl. Sol. Energy **58**, 323 (2022).
[13] I. Kaiser, K. Ernst, Ch. H. Fischer, R. Könenkamp, C. Rost, I. Sieber & M. C. Lux-Steiner, Sol. Energy Mater. Sol. Cells **67**, 89 (2001)
[14] T. K. Tulka, N. Alam, K. M. Elme & M. M.Hossain, Appl. Sol. Energy **58**, 28 (2022)
[15] A. Fujishima, X. T. Zhang, Proc. Japan Acad. **81**, 33 (2005).
[16] K. Ernst, A. Belaidi, R. Könenkamp, Semicond. Sci. Technol. **18**, 475 (2003).
[17] M. Nanu, J. Schoonman, A. Goossens, Adv. Func. Mater. **15**, 95 (2005).
[18] Wang Yu, Gong Hao, Fan Benhu, Guangxia Hu, J. Phys. Chem. **114**, 3256 (2010).
[19] A. Mittiga, E. Salza, F. Sarto, M. Tucci, R. Vasanthi, Appl. Phys. Lett. **88**, 163502 (2006).

[20] L. Olsen, F. Addis, W. Miller, Solar Cells **7**, 247 (1982).
[21] Y. Nishi, T. Miyata, T. Minami, J. Vac. Sci. Technol. A **30**, 04D103 (2012).
[22] T. Minami, Y. Nishi, T. Miyata, Appl. Phys. Express **6**, 044101 (2013).
[23] Y. S. Lee, D. Chua, R. E. Brandt, S. C. Siah, J. V. Li, J. P. Mailoa, S. W. Lee, R. G. Gordon, T. Buonassisi, Adv. Mater. **26**, 4704 (2014)
[24] A. S. Brown, M. A. Green, Physica E **14**, 96 (2002).
[25] E. Fortunato, V. Figueiredo, P. Barquinha, E. Elamurugu, R. Barros, G. Gonçalves, S.-H. K. Park, C.-S. Hwang, R. Martins, Appl. Phys. Lett. **96**, 192102 (2010).
[26] F. Anwar, S. SarwarSatter, R. Mahbub, S. Mahmud Ullah, S. Afrin, International Journal of Renewable Energy Research. **7**, 885 (2017).
[27] K. Decock, S. Khelifi, M. Burgelman, Thin Solid Films **519**, 7481 (2011).
[28] A. Niemegeers, M. Burgelman, Solar Cells **1**, 901 (1996).
[29] M. Burgelman, P. Nollet, S. Degrave, Thin Solid Films **361**, 527 (2000).
[30] P. Sawicka-Chudy, M. Sibiński, G. Wisz, E. Rybak-Wilusz, M. Cholewa, Journal of Physics **1033**, 012002 (2018).
[31] P. Sawicka-Chudy, Ł. Głowa, S. Z. Górny, G. Wisz, M. Sibiński, E. Rybak-Wilusz, P. Potera, J. Nanoelectron. Optoelectron. **13**, 715 (2018).
[32] A. K. Singh, R. Walia, M. S. Chauhan, R. S. Singh, V. K. Singh., Environ. Sci. Pollut. Res. **30**, 98718 (2023)
[33] N. Rahman, M. D. Haque, M. F. Rahman, M. M. Islam, M. Airin Nahar Juthi, A. Rani Roy, M. Alema Akter, M. Foridul Islam, Discov. Mater. **3**, 25 (2023)

*Corresponding author: beddiaf.zaidi@univ-batna.dz