JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. 11 No 2, 02030(4pp) (2019) ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том 11 № 2, 02030(4cc) (2019)

# Role of TCO Films in Improving the Efficiency of $CdS/MoS_2$ Heterojunction Solar Cells

B. Zaidi[1,*], M.S. Ullah[2], B. Hadjoudja[3], S. Gagui[3], N. Houaidji[3], B. Chouial[3], C. Shekhar[4]

[1] *Department of Physics, Faculty of Material Sciences, University of Batna 1, Batna, Algeria*
[2] *Department of Electrical and Computer Engineering, Florida Polytechnic University, Lakeland, USA*
[3] *Laboratory of Semiconductors, Department of Physics, University of Badji-Mokhtar, Annaba, Algeria*
[4] *Department of Applied Physics, Amity University Gurgaon, Haryana, 122413 India*

(Received 17 December 2018; revised manuscript received 02 April 2019; published online 15 April 2019)

Thin film solar cell is a second generation solar cell that is made by depositing one or more thin layers. Debutant analysis of the parameters impeding the efficiency of the $CdS/MoS_2$ heterojunction based photovoltaic device is the chief novelty of the present report. In this work, we investigated the effect of Transparent Conductive Oxide (TCO) utilizing zinc oxide (ZnO) or lead oxide (PbO) antireflective thin film (ARC) on the characteristics of $CdS/MoS_2$ heterojunction solar cell (short circuit current density $J_{sc}$, open circuit voltage $V_{CO}$, power-voltage (*P-V*) and capacitance-voltage (*C-V*)). All these options are implemented in the one-dimensional numerical simulation program SCAPS.

The results obtained show that as a result of the use of TCO, the short circuit current density $J_{sc}$ decreases as a function of the applied voltage for both cells. The decrease in the current density is modest below 0.6 V and sharper above. On the other hand, the power density increases almost linearly to a maximum of ~ 3.83 and 3.29 mW/cm² for ZnO and PbO TCO, respectively. The variation in the capacitance with the voltage is similar to the variation of the current density for both configurations and we found that the efficiency of ZnO coating solar cells is higher than of cells coated with PbO.

**Keywords:** $CdS/MoS_2$, Zinc oxide, Lead oxide, Solar cells, Capacitance-voltage, SCAPS-1D.

DOI: 10.21272/jnep.11(2).02030 PACS numbers: 84.60.Jt, 88.40.jm

## 1. INTRODUCTION

Photovoltaic cell is a large cell that consists of one layer of P-type and another layer of N-type to form a PN junction and converts solar energy to electricity by photovoltaic effect. Currently, we have Si-technology based conventional solar cell in the form of monocrystalline, polycrystalline, amorphous or thin film, dye sensitized, ionic dye sensitized. However, according to report that produced by T. Tiedje [1-4], the theoretical limitation of efficiency of silicon based solar cell is 29.8 % (~ 30 %) due to poor absorption of total incident light as a lack of completely transparent surface and inappropriate band gap material, and low reflection within the device causing faster recombination of emitted electrons. Currently, the 90 % market share is occupied by silicon based solar cells but hasn't been able to provide the solution of the challenging question of increasing efficiency above 30 % [5-7]. As a result, tandem cell is constructed from single junction GaAs and multi-junction (up to three p-n junctions) concentrators with different materials to absorb a larger spectrum of incident light. However, the reported theoretical efficiency is 40.8 % under concentrations of 326 suns, which is not true for practical conditions [8-10]. In reality, the efficiency drop to 33.8% with one sun and the process itself is not matured like Si-based technology [11, 12].

Further, there has been a chain of studies [13-15] on carbon nanotubes (CNTs) as a prospective material that can be used to improve the solar cell efficiency due to the following reasons: (i) CNT films create multiple heterojunctions and add more band gaps; (ii) Nanocomposite-semiconductor heterojunctions ensure more photo-current; (iii) CNTs are more transparent; (iv) CNTs can be very good electrical conductors; and (v) CNTs are known to be electrochemically very active. CNTs also have been explored as a possible replacement of Cu interconnects [14]. This means that CNTs have already begun interaction with Si and other IC technologies. Therefore, the probability of succeeding in integrating CNTs in solar cells is promising. A single SWCNT as a photodiode that can be used as a rudimentary solar cell demonstrated by the Cornell group [12]. A conceptual PV device with vertically aligned SWCNTs is used as a photoactive material. The tubes are contacted between two different types of metal electrodes and an electric field of incident light is polarized parallel to the nanotube axis [12]. A different concept of a PV device with SWCNTs nanowelded onto palladium (Pd) and aluminum (Al) electrodes that are patterned on Si wafers with a thermally oxidized layer [13]. The overall efficiency could be achieved only 7 %-8 %. However, these investigations identify the research challenges in the anticipated new direction for solar cell technology. Therefore, there has been a significant concern to find an alternative solution for crossing the efficiency barriers of current solar cells due to the increasing energy needs for efficient and high performance consumer electronics.

Recent researches indicate that molybdenum disulfide ($MoS_2$) which is one of the transition-metal dichalcogenides (TMDs) material in which d-electron interactions can give rise to new physical phenomena. It shows very promising properties for not only future nanoscale device applications [16], but also for numerous photonic applications such as light emitter, photodetectors, and solar cells. It is also considered as the new super material that replaces conventional silicon, semiconductor

* zbeddiaf@gmail.com

 

III-V materials and even graphene in the next generation nanoelectronic devices due to its unique set of material, electrical and optical properties. Bulk $MoS_2$ is an indirect gap semiconductor with a bandgap in the near-infrared frequency range, and $MoS_2$ mono-layer is a direct gap semiconductor with a bandgap in the visible frequency range [16]. In general, this unique property of $MoS_2$ and 2D materials enables the creation of atomically smooth material sheets and the precise control on its number of molecular layers. The indirect to direct crossover occurs at the mono-layer limit resulting in strong contrast in photoluminescence efficiency between mono- and multi-layer sheets.

CdS/$MoS_2$ films create multiple heterojunctions and add more bandgaps. Due to the presence of these heterojunctions, absorbed light bounces around for longer time inside the cell, giving more time to deposit photon energy and produce electric current. Therefore, in this work, it is provided an in depth acquaintance to the new technological advancement in the field of solar cells. The use of a possible combination of CdS/$MoS_2$ heterojunction with ZnO or PbO is proposed as a probable step to increase the solar cell efficiency above the theoretical limit.

The rest of the paper is organized as follows. Section 2 provides material parameters with the structure of solar cell. Simulation results are discussed in Section 3. Finally, Section 4 concludes the paper with a brief description of further research directions.

## 2. MATERIAL PARAMETERS

The proposed device structure of solar cell is shown in Fig. 1. The composition of CdS/$MoS_2$ heterojunction solar cell from top to bottom in the cells is composed of a transparent conductive film of zinc oxide (ZnO) or lead oxide (PbO); CdS/$MoS_2$ layers in the sequence, N-type then P-type; and a Mo/glass substrate.

| |
|---|
| ZnO or PbO |
| CdS |
| $MoS_2$ |
| Mo/glass |

**Fig. 1**– Structure of solar cell

The parameters used for simulations of CdS/$MoS_2$ heterojunction solar cell are summarized in Table 1. All simulations in this work were performed under ambient temperature (300 °K).

This numerical study was employed by means of Solar Cell Capacitance Simulator structures (SCAPS-1D) software [17, 18] to analyze the CdS/$MoS_2$ heterojunction solar cells. This computer simulation program was developed by the Department of Electronics and Information Systems (ELIS), University of Gent, Belgium. It has been extensively tested in solar cells by M. Burgelman et al. [19, 20]. SCAPS is capable of solving the basic semiconductor equations, the Poisson equation and the continuity equations for electrons and holes. SCAPS calculates the solution of the basic semiconductor equations in one-dimensional and in steady state conditions.

SCAPS analyzes the physics of the model and explains the recombination profiles, electric field distribution, carrier transport mechanism and individual current densities. The continuity equations for electrons and holes are:

$$\begin{cases} J_n = qn\mu_n \dfrac{\partial \varphi}{\partial x} + qD_n \dfrac{\partial n}{\partial x} \\ J_p = -qp\mu_p \dfrac{\partial \varphi}{\partial x} + qD_p \dfrac{\partial p}{\partial x} \end{cases}$$

where $D_n$ is the electron diffusion coefficient, $D_p$ is the hole diffusion coefficient, $\mu_n$ is the electron mobility, and $\mu_p$ is the hole mobility.

Poisson's equation is used to describe the relationship between potential and space charges, as shown:

$$\frac{\partial^2}{\partial x^2}\varphi(x) = \\ = \frac{q}{\varepsilon}\left[ n(x) - p(x) - N_D^+(x) + N_A^-(x) - p_t(x) + n_t(x) \right]$$

where $\varphi$ is the electrostatic potential, $q$ is the elementary charge, $\varepsilon$ is the permittivity, $n$ is the density of free electrons, $p$ is the density of free holes, $N_D^+$ is the ionized donor-like doping density, $N_A^-$ is the ionized acceptor-like doping density, $p_t$ is the trapped hole density, $n_t$ is the trapped electron density. The continuity equations for electrons and holes are:

$$\begin{cases} \dfrac{\partial J_n}{\partial x} = G - R \\ \dfrac{\partial J_p}{\partial x} = G - R \end{cases}$$

where $J_n$ and $J_p$ are electron and hole current densities, $R$ is the recombination rate, and $G$ is the generation rate.

**Table 1** – Physical parameters used in our simulation

| Parameters | $MoS_2$ | CdS | ZnO | PbO |
|---|---|---|---|---|
| Thickness(nm) | 400 | 20 | 200 | 200 |
| Electron affinity (eV) | 4.22 | 4.2 | 4.6 | 4.5 |
| $E_g$ (eV) | 1.8 | 2.45 | 3.3 | 2.5 |
| $N_d$ ($cm^{-3}$) | $10^6$ | $10^{17}$ | 2.2 $10^{18}$ | 2.2 $10^{18}$ |
| $N_a$ ($cm^{-3}$) | $10^{17}$ | $10^6$ | 1.8 $10^{19}$ | 1.8 $10^{19}$ |

## 3. RESULTS AND DISCUSSION

Fig. 2 reflects the change in the current density as a function of voltage. The current decreases with TCO coating as the voltage increases.

The initial decreasing rate up to 0.6 V is slow, however, after that the decreasing rate is more rapid, which clearly reflects the relationship between the electrical field and voltage.

On the other hand, Fig. 3 shows the variation of power generated by the two different configurations of the solar cell as a function of voltage. As seen from Fig. 3, the power density increases linearly to a maximum of ~ 3.83 and 3.29 mW/$cm^2$ for ZnO and PbO, respectively.

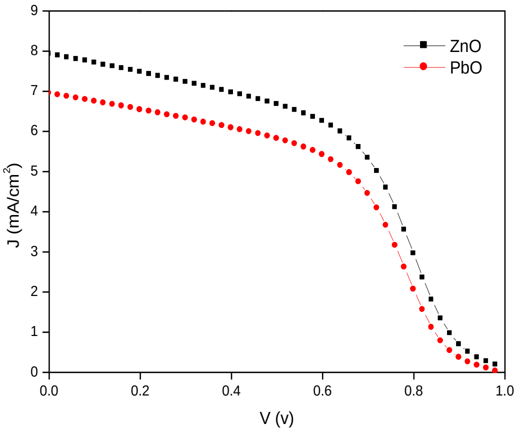


**Fig. 2** – Effect of TCO coating on J(V) characteristics

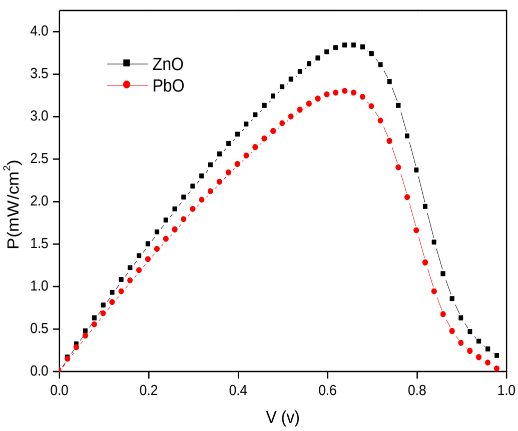


**Fig. 3** – Effect of TCO coating on P(V) characteristics

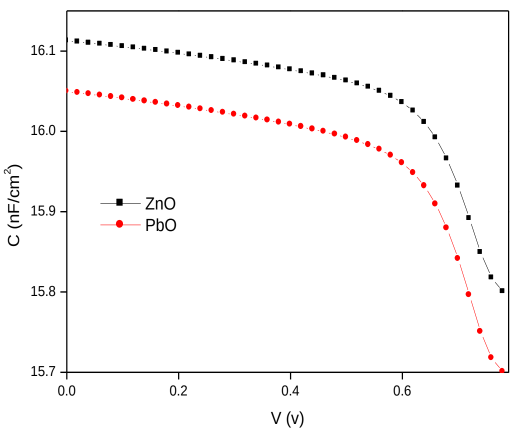


**Fig. 4** – Effect of TCO coating on C(V) characteristics

**Table 2** – Solar cell performance parameters calculated with SCAPS-1D ($ZnO/CdS/MoS_2$ and $PbO/CdS/MoS_2$)

| | $ZnO/\ CdS/MoS_2$ | $PbO/\ CdS/MoS_2$ |
|---|---|---|
| Isc ($mA/cm^2$) | 7.98 | 6.99 |
| Voc (v) | 1.2 | 1.04 |
| FF (%) | 47.51 | 48.14 |

The performance parameters of the two configurations of the solar cell are presented in Table 2.

Fig. 4 illustrates the variation of the capacitance of the two configurations. The variation of the capacitance with the voltage is similar to the variation of the current density as presented above in Fig. 3. It is observed that the capacitance is larger for the solar cell with ZnO transparent layer due to the lower charge carrier concentration in the layer.

Fig. 5 shows the efficiency as a function of light power with the presence of ZnO or PbO. When the incident light power is in the range of 400 and 1000 $W/m^2$, the efficiency of solar cell increases more than 1 % with the presence of ZnO compared to PbO. With the incident light power of 200 $W/m^2$, the efficiency increases almost 3 % when ZnO is instead of PbO.

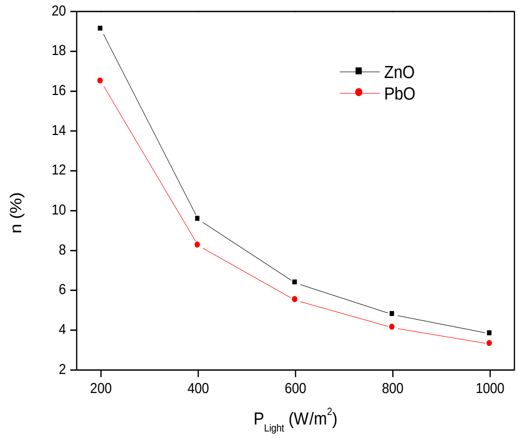


**Fig. 5** – Efficiency as a function of light power

## 4. CONCLUSIONS

This research paper investigates the progress, challenges and opportunities on the existing and new solar cells to improve the efficiency of solar cells and photovoltaic devices. Molybdenum disulphide ($MoS_2$) with ZnO or PbO have been proposed as the potential materials that could significantly improve the solar cell efficiency. Thin film $CdS/MoS_2$ technology has been discussed in detail. The discussion points out various improvements in the solar industry and the available technologies and new methods to achieve the higher efficiency and performance of solar cells. This investigation provides one alternative solution and identifies the current research challenges that are anticipated new direction for solar cell technology.

## ACKNOWLEDGEMENTS

We gratefully acknowledge to Dr. Marc Burgelman, University of Gent, Belgium, for providing the SCAPS-1D simulation software.

## REFERENCES


1. J. Nelson, *The Physics of Solar Cells* (London: Imperial College Press: 2003).
2. B. Zaidi, S. Belghit, C. Shekhar, M. Mekhalfa, B. Hadjoudja, B. Chouial, *J. Nano- Electron. Phys.* **10**, 05045 (2018).
3. B. Zaidi, B. Hadjoudja, H. Felfli, B. Chouial, A. Chibani, *Revue de Métallurgie* **108**, 443 (2011).
4. B. Zaidi, B. Hadjoudja, B. Chouial, K. Kamli, A. Chibani, C. Shekhar, *Silicon* **10**, 2161 (2018).
5. T. Tiedje, E. Yablonovitch, G. Cody, B.G. Brooks, *IEEE T. Electron Dev.* **31**, 711 (1984).
6. B. Zaidi, B. Hadjoudja, B. Chouial, S. Gagui, H. Felfli, A. Chibani, *Silicon* **7**, 275 (2015).
7. B. Zaidi, I. Saouane, C. Shekhar, *Silicon* **10**, 975 (2018).
8. A. Slaoui, R.T. Collins, *MRS Bull.* **32**, 211 (2007).
9. B. Zaidi, B. Hadjoudja, C. Shekhar, B. Chouial, R. Li, M.V. Madhava Rao, S. Gagui, A. Chibani, *Silicon* **8**, 513 (2016).
10. B. Zaidi, B. Hadjoudja, H. Felfli, A. Chibani, *Turk. J. Phys.* **35**, 185 (2011).
11. B. Zaidi, B. Hadjoudja, B. Chouial, S. Gagui, H. Felfli, A. Magramene, A. Chibani, *Silicon* **7**, 293 (2015).
12. B. Zaidi, S. Belghit, C. Shekhar, B. Hadjoudja, B. Chouial, *Nanosistemi, Nanomateriali, Nanotehnologii* **16**, 713 (2018).
13. C. Chen, L. Yang, Y. Lu, G. Xiao, Y. Zhang, *IEEE T. Nanotechnol.* **8**, 303 (2009).
14. K. Banerjee, N. Srivastava, *IEEE/ACM Design Automation Conference*, 809 (2006).
15. S.A.M. Albathi, N. Ahmed, *AIP Conf. Proc.* **2083**, 020005 (2019).
16. M.S. Ullah, A.H. Yousuf, A.D. Es-Sakhi, M.H. Chowdhury, *AIP Conf. Proc.* **1957**, 020001 (2018).
17. J. Verschraegen, M. Burgelman, *Thin Solid Films* **515**, 6276 (2007).
18. K. Decock, S. Khelifi, M. Burgelman, *Thin Solid Films* **519**, 7481 (2011).
19. M. Burgelman, P. Nollet, S. Degrave, *Thin Solid Films* **361**, 527 (2000).
20. M. Burgelman, J. Verschraegen, S. Degrave, P. Nollet, *Prog. Photovolt.: Res. Appl.* **12**, 143 (2004).


## Роль плівок ППО у підвищенні ефективності сонячних елементів на основі гетеропереходів $CdS/MoS_2$


B. Zaidi[1], M.S. Ullah[2], B. Hadjoudja[3], S. Gagui[3], N. Houaidji[3], B. Chouial[3], C. Shekhar[4]

[1] *Department of Physics, Faculty of Material Sciences, University of Batna 1, Batna, Algeria*
[2] *Department of Electrical and Computer Engineering, Florida Polytechnic University, Lakeland, USA*
[3] *Laboratory of Semiconductors, Department of Physics, University of Badji-Mokhtar, Annaba, Algeria*
[4] *Department of Applied Physics, Amity University Gurgaon, Haryana, India 122413*



Тонкоплівковий сонячний елемент є сонячним елементом другого покоління, який виготовляється шляхом нанесення одного або більше тонких шарів. Головною новизною даної роботи є вперше зроблений аналіз параметрів, що перешкоджають ефективності фотоелектричного пристрою на основі гетеропереходу $CdS/MoS_2$. У роботі досліджено вплив прозорого провідного оксиду (ППО) з використанням тонкої плівки оксиду цинку ZnO або оксиду свинцю PbO на характеристики сонячних елементів гетеропереходу $CdS/MoS_2$ (щільність струму короткого замикання $J_{SC}$, напруга розімкнутого ланцюга $V_{CO}$, потужність-напруга (*P-V*) і ємність-напруга (*C-V*)). Усі ці характеристики реалізовані в одновимірній програмі чисельного моделювання SCAPS.

Отримані результати показують, що в результаті використання ППО, щільність струму короткого замикання $J_{SC}$ зменшується як функція прикладеної напруги для обох елементів. Незначне зниження щільності струму відбувається нижче 0.6 В і суттєве – вище цієї напруги. З іншого боку, щільність потужності зростає майже лінійно до максимуму ~ 3.83 і 3.29 мВт/см² для ZnO і PbO TCO, відповідно. Зміна ємності з напругою аналогічна зміні щільності струму для обох конфігурацій, і було виявлено, що ефективність сонячних елементів з покриттям ZnO вище, ніж елементів, покритих PbO.



**Ключові слова:** $CdS/MoS_2$, Оксид цинку, Оксид свинцю, Сонячні елементи, Ємність-напруга, SCAPS-1D.