

Simulation and Optimization of ZnO/CuO/Cds Solar Cell Using SCAPS

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Received: October 11, 2023

Accepted: December 19, 2023

Published: December 22, 2023

Citation: Chandran I, Subash TD, Batumalay M. 2023. Simulation and Optimization of ZnO/CuO/Cds Solar Cell Using SCAPS. *NanoWorld J* 9(S5): S97-S100.

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Abstract

Here, SCAPS-1D (Solar Cell Capacitance Simulator) software was used for simulations of ZnO (Zinc oxide)/CuO (Copper oxide)/Cds (Cadmium sulfide) thin-film solar cells. Based on the device structure and manufacturing process, the solar cell structure parameters such as CuO layer thickness, ZnO layer, etc. were evaluated in detail. The results showed that the optimal structure of the ZnO/CuO/Cds heterojunction solar cell thin film could be obtained when the ZnO layer thickness, the CuO layer and the Cds layer of the buffer layer are 0.1 μm , 2 μm and 1 μm . Thin-film solar cells have been widely used for power generation due to their low manufacturing cost and high conversion efficiency. ZnO is a highly conductive and excellent transparent thin film in the visible region. Simulation results of this three-layer heterojunction layer indicate that a high efficiency (η) value of 18.61 can be obtained at a short-circuit current density as high as 36.323 $\text{mA}\cdot\text{cm}^{-2}$.

Keywords

SCAPS-1D, Zinc oxide, Copper oxide, Cadmium sulfide, Heterojunction solar cell

Introduction

A nation's ability to grow economically and socially depends on its access to energy. The basic goal of energy transformation is access to energy to increase productivity and quality of life. Much energy is currently produced on a large scale from many sources, including fossil fuels, wind turbines, etc. [1, 2]. However, the continued use of fossil fuels is not environmentally friendly due to the greenhouse gas emissions they produce. In addition to the direct impact on agricultural activities and overall health, access to electricity is critical to achieving the Sustainable Development Goals. As such, countries must consider measures to ensure uninterrupted power supply.

The use of renewable energy technologies such as solar energy is appropriate to meet this demand. Solar energy was a renewable source of energy and could not be destroyed. Solar cells have been used as an important solution to meet the energy shortage and also to reduce the environmental problems arising from the use of fossil fuels [1]. The use of solar cells to generate electricity from incident sunlight has improved the conduct of research in various fields. An important area of research in this area is the design of solar cells. Both chemical and physical properties affect their energy efficiency. Examples of physical properties of solar cells are density, temperature, and thickness [1]. The simulation was used to optimize the parameters that affect the production of electricity from solar energy.

The design of potential photovoltaic materials focuses on solving the problems of realizing high energy efficiency, low cost, and stability. Realization of these performance goals should be considered during the doping of semiconductors used in solar cell design. Suitable semiconductors for the design of high-power solar cells can be realized from unconventional doping of p-n type layered material. All potential alternative photovoltaic materials that have been introduced recently must meet three main properties: high efficiency, low cost, and stability. In the last few years, it has been the subject of extensive research due to its great potential for the production of highly efficient solar cells.

Materials and Method

Solar cell structure

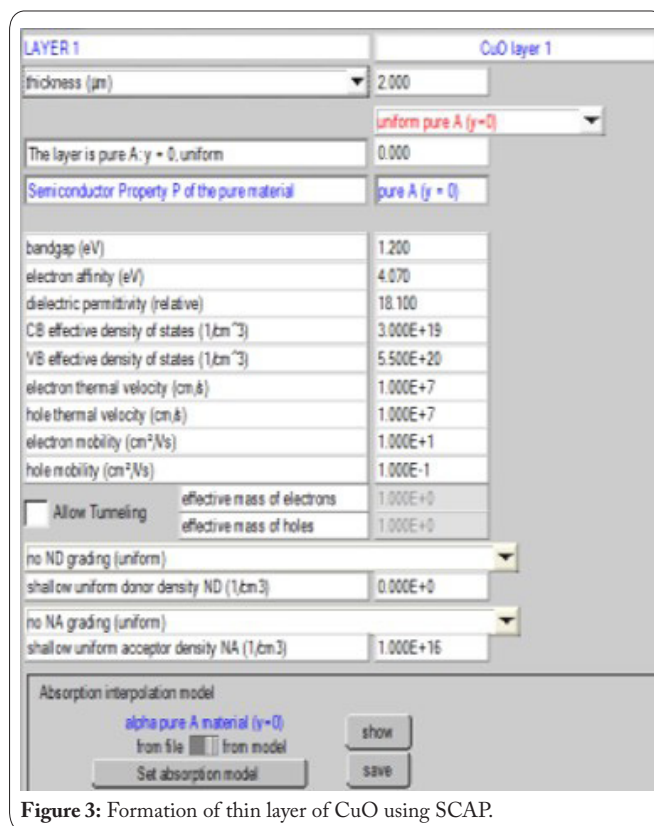
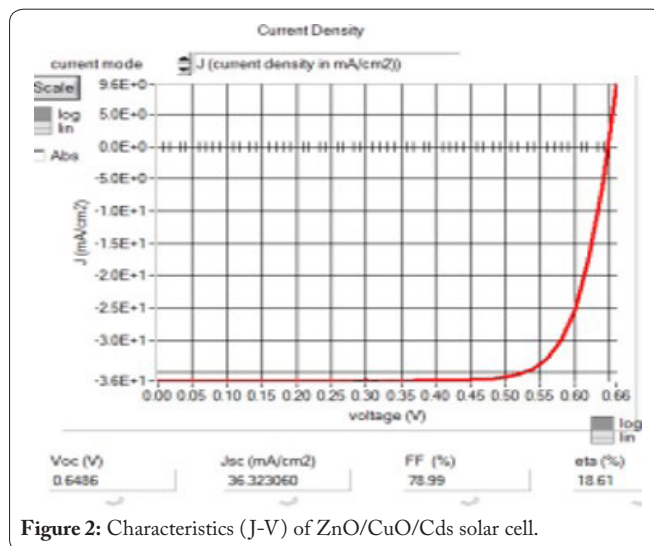
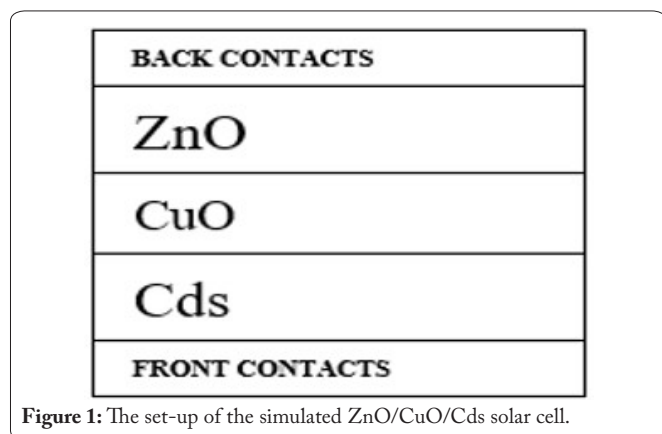
The simulation of thin-film planar ZnO/CuO/Cds heterojunction solar cells was performed without the introduction of additional defects. The thickness of each layer was controlled as 0.1 μm, 2 μm, and 1 μm for ZnO, CuO, and Cds layers, respectively. The density of shallow donors in the ZnO layer was determined to be 1016 cm⁻³. The shallow acceptor densities in CuO and Cds were set to 1016 cm⁻³ and 1015 cm⁻³, respectively. Based on this structure, a short circuit current density of up to 36.323 mA.cm⁻² can be obtained, resulting in an energy conversion efficiency of 18.61%. Figure 1 presents the set-up of the simulated ZnO/CuO/Cds solar cell.

It could be concluded that this ZnO/CuO/Cds thin-film planar heterojunction structure works well in the photoconversion process for solar cells. In the following section, based on the structure of the ZnO/CuO/Cds heterojunctions, the influence of the thickness of the ZnO, CuO and Cds layers, and temperature fluctuations and CuO concentration can be observed.

Simulation of a thin film plane

The thickness of the ZnO and CuO layers, the shallow donor density in the Cds layer, which can be controlled by actual device fabrication processes, will be evaluated using different approaches to find the optimal structure. Figure 2 presents characteristics (J-V) of ZnO/CuO/Cds solar cell.

Figure 3 shows the common features for producing a thin uniform layer of CuO. To make a p-type semiconductor such as CuO, the electron affinity is 4.07 eV, and the band gap



energy is 1.2 eV. The thickness varies from 0.5 μm to 2 μm. The effective density of states CB (conductance band) and VB (valence band) must be 3.00E+19 and 5.5E+20. Electron and hole thermal velocity can be 1000E+8 cm/s. Electron and hole affinity values are constant. The electron mobility can be 10 and the hole mobility can be 0.1. The dielectric permittivity is 18.10.

Likewise for manufacturing the layer of an n-type material like ZnO, the following properties should be maintained. The electron affinity be 3.9 eV and band gap energy be 3.37 eV. The thickness varies from 0.05 μm to 0.1 μm. CB and VB effective density of states must be 1.32E+20 and 1.500E+21. The electron and hole thermal velocity may be 1.000E+8 cm/s. The electron mobility may be 20 and hole mobility may be 10. The dielectric permittivity is 86.

For manufacturing the buffer structure like Cds, following properties must be noted. The electron affinity be 4.5 eV and band gap energy be 2.4 eV. The thickness varies from 0.5 μm to 1 μm . CB and VB effective density of states must be $2.2\text{E}+18$ and $1.900\text{E}+19$. The electron and hole thermal velocity may be $1.000\text{E}+8$ cm/s. The electron mobility be 350 and hole mobility may be 25. The dielectric permittivity is 10. In between two layers the intrinsic layer was added.

Properties of the materials

Parameters for Cds, CuO, and ZnO used in simulations are shown in table 1 [3]. Table 2 lists the parameters used in the rear and front contacts [4]. The effects of CuO and ZnO layer thickness were analyzed. Finally, based on the optimized ZnO/CuO/Cds thin-film planar heterojunction solar cell structure, the cell performance at individual solar concentrations and operating temperatures was also investigated.

Table 1: The properties of ZnO, CuO, and Cds layers.

Parameter	ZnO	CuO	Cds
Thickness, d (μm)	0.1	2	1
Bandgap, Eg (eV)	3.37	1.2	2.4
Electron affinity (eV)	3.9	4.07	4.5
Relative permittivity	86	18.1	10
Conduction band effective density of states, NC (cm^{-3})	$1.320\text{E}+21$	$3.00\text{E}+19$	$2.2\text{E}+18$
Valance band effective density of states, NV (cm^{-3})	$1.5\text{E}+20$	$5.50\text{E}+20$	$1.9\text{E}+19$
Electron mobility	20	10	350
Hole mobility	10	0.1	25
Shallow uniform donor density, ND (cm^{-3})	$1.000\text{E}+19$	0	$1.000\text{E}+17$
Shallow uniform acceptor density, NA (cm^{-3})	0	$1.000\text{E}+16$	0

Table 2: Parameters of back and front contacts that used in SCAPS simulation.

Interface parameter	Front contacts	Back contacts
Metal work function (eV)	4.472	5.297
Surface recombination velocity of holes (cm.s^{-1})	10^7	10^7
Surface recombination velocity of electrons (cm.s^{-1})	10^7	10^7

Results and Discussion

The effect of varying temperature

The efficiency and performance of the photovoltaic cell structure are affected by a number of factors. The cause is the result of a demanding internal physical process. We need to simulate and evaluate different attributes as well as different potential circumstances to gain confidence in the solar cell model. Temperature plays an important role for various parameters of solar cells. Figure 4 shows the sample graph to show the effect of temperature on the J (V) characteristics. It is clear that increasing the temperature leads to an inevitable decrease of the voltage. The optimum temperature for this study is 300 K. In this work, the temperature can be varied from (280 K - 360 K). It should be noted that the overall efficiency (Eta) is affected by temperature (Figure 5). As the

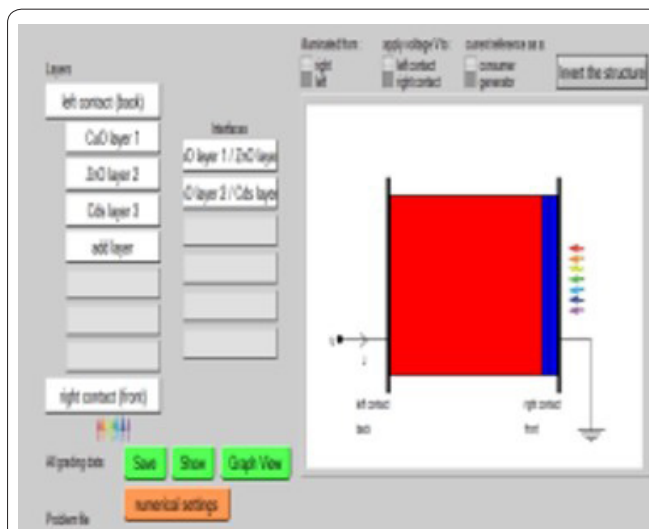


Figure 4: Heterojunction solar cell structure using ZnO/CuO/Cds.

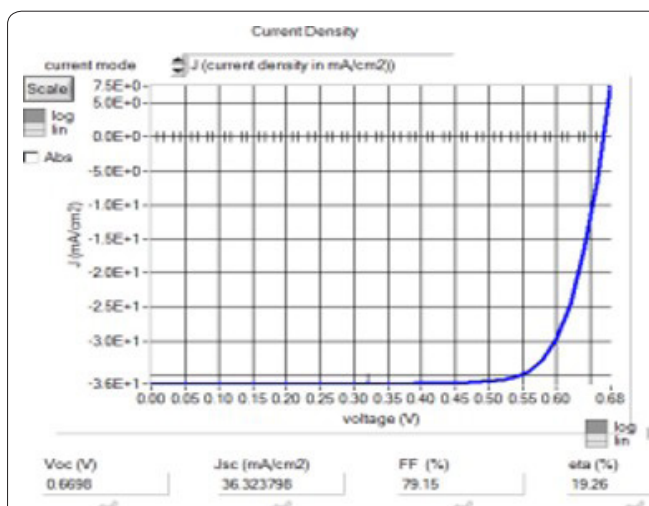


Figure 5: Variation of value of efficiency (Eta) at 280 K.

temperature increases, the efficiency value decreases (Table 3).

The effect of varying bandgaps of ZnO

The efficiency and performance of the photovoltaic cell structure are affected by a number of factors. The cause is the result of a demanding internal physical process. We need to simulate and evaluate different attributes as well as different potential circumstances to gain confidence in the solar cell model. Here we consider the bandgap variation of ZnO solar cells. The bandgap of ZnO ranges from 3.10 eV to 3.37 eV (Figure 6). The J_{sc} parameter of the thin-film planar ZnO/CuO/Cds heterojunction solar cell increases slightly with the increase of the donor bandgap and almost saturates at higher values. However, the V_{oc} value hardly changed [5]. Table 4

Table 3: Variation of temperature and its efficiency.

Temperature	V_{oc}	J_{sc}	FF	Eta
260	0.6733	36.3239	79.23	20.13
280	0.6698	36.3237	79.15	19.26
300	0.6486	36.3230	78.99	18.61
320	0.6061	36.3243	77.78	17.12
340	0.5633	36.319	76	15.55

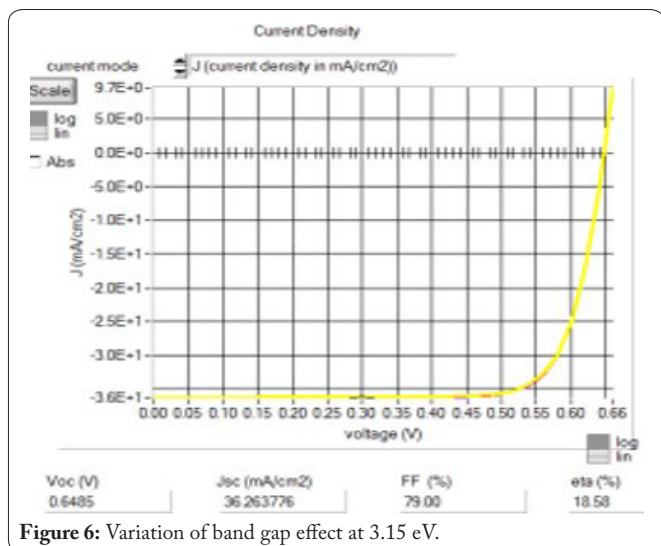


Figure 6: Variation of band gap effect at 3.15 eV.

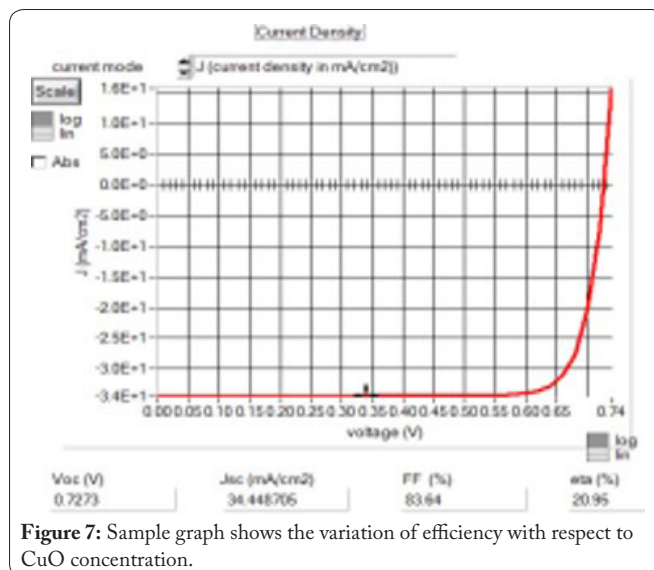


Figure 7: Sample graph shows the variation of efficiency with respect to CuO concentration.

Table 4: Variation of bandgap of ZnO.

Bandgap (eV)	V_{OC}	J_{SC}	FF	Eta
3.10	0.6485	36.263	79	18.58
3.15	0.6485	36.27449	78.99	18.58
3.20	0.6486	36.2897	78.99	18.59
3.30	0.6486	36.3103	78.99	18.60
3.37	0.6456	36.3230	78.99	18.61

Table 5: Variation due the concentration of CuO layer.

Concentration	V_{OC}	J_{SC}	FF	Eta
1.000E+13	0.6098	30.277218	41.91	7.74
1.000E+15	0.6156	35.8762	51.97	11.48
1.000E+16	0.6486	36.3230	78.99	18.61
1.000E+18	0.7273	37.448	83.64	20.95

shows the variations in values of V_{OC} , J_{SC} , FF, and Eta with respect to the bandgap of ZnO.

The effect of varying concentration of CuO

In this work, the value of CuO concentration varies (Figure 7). And the following changes can be observed by changing the concentration. CuO is inherently a p-type material, and the carrier concentration depends on the defects in the synthetic material. Table 5 shows that as the concentration of CuO increases, the efficiency of the solar cell also increases [3]. The carrier concentration in the CuO layer ranges from 10^{12} to 10^{18} cm^{-3} . The efficiency begins to increase with increasing concentration [6]. Table 5 shows the variation of V_{OC} , J_{SC} , FF, and Eta values with respect to the carrier concentration in the CuO layer. It is clearly mentioned that the value of efficiency slightly increases with bandgap.

Conclusion

In conclusion, ZnO/CuO/Cds heterojunction solar cells were simulated using SCAPS 1D software. After a successful simulation process, parameters such as the highest η of 18.61% with a V_{OC} value of 0.6486 V, a J_{SC} value of 36.323060 mA/cm² and an FF value of 78.99% were realized at the optimal temperature of 300 K. from another study we observed that the efficiency decreases with increasing temperature. which means that the temperature is inversely proportional to the overall efficiency of the solar cells. We also changed the bandgap of an n-type material such as ZnO. It follows that the band gap slightly increases efficiency. When the concentration of the CuO carrier changes, it shows an inevitable increase in efficiency. V_{OC} , J_{SC} , and FF values also change with variation of carrier concentration, temperature, and bandgap.

Acknowledgements

None.

Conflict of Interest

None.

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