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Insight of ZnO/CuO and ZnO/Cu_2O solar cells efficiency with SCAPS simulator

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Abstract

Despite the low power conversion efficiency of solar cells n-ZnO/p-CuO and n-ZnO/p-Cu_2O, they can contribute to the development of photovoltaic energy. To optimize their yields, the simulator software SCAPS-1D was used in this work to do the simulations of the two cells (Fig. 1) by varying certain parameters. Its parameters were thickness, band-gap, shallow uniform donor density (ND) for the ZnO, and shallow uniform acceptor density (NA) for the CuO and Cu_2O. The values optimized of these parameters gave short-circuit currents and efficiencies of 27.7755 mA.cm^{-2}, 31.40%, and 12.9790 mA.cm^{-2}, 13.34% respectively for the solar cells n-ZnO/p-CuO and n-ZnO/p-Cu_2O (Fig. 2). Our results reveal that the n-ZnO/p-CuO solar cell is more efficient than the n-ZnO/p-Cu_2O solar cell and can be used for converting solar energy into electricity.

Graphical abstract

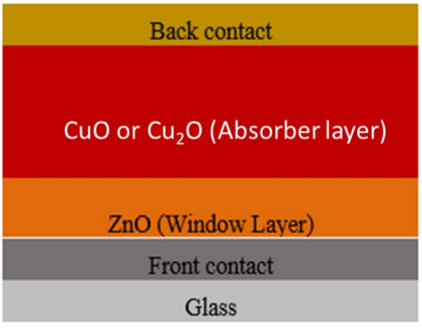

Figure 1

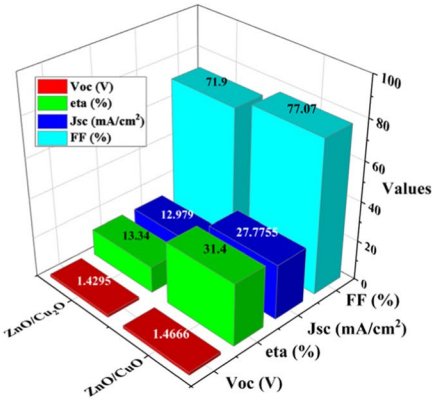

Figure 2

Keywords Oxide · Efficiency · Solar cells · Simulation · SCAPS

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1 Introduction

The world evolves with all the technology in it. Solar energy is not on the sidelines. In fact, silicon has been the subject of research for several years and is gradually giving way to other semiconductors such as oxides (Li et al. 2017; Bouich 2021; Lu et al. 2016; Shen et al. 2015; Wisz et al. 2018). Several works in the literature have been realized on the copper oxide and zinc oxide used in solar cells (Fortunato et al. 2007). Apart from solar cells made of several types of materials (Tsunomura et al. 2009; Khan et al. 2018; Ajmal Khan and Suemasu 2017), There are heterojunction solar cells made only of metal oxides. The oxides being abundant and less expensive, these cells called all-oxide photovoltaic cells are thus produced at low cost and can be an alternative to the high price of the solar cells generally used. This has prompted the scientific community to take an interest in these types of photovoltaic solar cells (Morasch et al. 2014; Wisz et al. 2018; Ruhle et al. 2012). ZnO/CuO and ZnO/Cu_2O n-p junction have good properties for optoelectronic applications and can be competitive in the solar cell market (Mizuno et al. 2020).

ZnO is a cheap and abundant material in nature. Its properties such as its transparency in the visible and its direct bandgap of 3.3 eV make it a good candidate for electronic and optoelectronic applications (Mizuno et al. 2020; Mahajan et al. 2020). Due to its properties, cupric oxide (CuO) is used as an active layer in solar cells. In fact, it is a p-type semiconductor stable, cheap, and non-toxic with a bandgap of 1.2 eV (Kidowaki et al. 2012). It has a monoclinic crystalline structure with an absorption coefficient of 105 cm^{-1} and its electrical resistivity varies from 10 to 105 cmΩ (Shabu et al. 2015; Ooi et al. 2013; Valladares et al. 2012; Liu et al. 2011).

This work is a theoretical study that uses the SCAPS-1D simulation program to simulate solar cells n-ZnO/p-CuO and n-ZnO/p-Cu_2O. The influence of certain parameters of the different layers on the performance of solar cells is studied. The goal of this work is therefore to optimize the values of these parameters to have the best efficiencies for the solar cells as well as to compare the performance of the two cells.

2 Simulator program SCAPS-1D

Several simulation software is used in the literature for thin film solar cells simulation (Decock et al. 2011) such as AMPS (Matin et al. 2010), ASPIN (Vukadinoyic et al. 2003), AFORS-HET (Froitzheim et al. 2003), and SCAPS-1D (Doumbia et al. 2022). We have used SCAPS-1D in this work. SCAPS-1D is a software simulation developed in Belgium at Gent University and was usable since 1998. Different characteristics of I-V, C-V, C-f, QE, band diagrams, electric field, carrier densities, and partial recombination currents can be used to show the results of the simulation. Before the simulation, the material parameters can be set as well as other parameters in the software such as temperature, voltage, frequency, and illumination. A stack of layers constitutes the cell. Each layer has a parameter entry. The front and the back contact are provided by two additional layers that already exist in the device (Sawicka-Chudy et al. 2018).

Table 1 Parameters of ZnO, CuO, and Cu_2O (Sawicka-Chudy et al. 2018; Lam 2020; Anwar et al. 2017; Gou and Murphy 2003; Wang et al. 2002; Xing et al. 2011; Scanlon et al. 2009)

Parameters	n-ZnO	p-CuO	p-Cu_2O
Thickness d (nm)	Varied	Varied	Varied
Bandgap E_g (eV)	Varied	Varied	Varied
Electron affinity E_A (eV)	4.30	4.07	3.20
Relative dielectric permittivity $\varepsilon_{n\text{-}p}$	9.00	18.10	7.11
Conduction band effective density of states N_C (cm^{-3})	2.2E+18	1.0E+19	2.0E+17
Valence band effective density of states N_V (cm^{-3})	1.8E+18	5.5E+20	1.1E+19
Electron mobility ($cm^2V^{-1}\ s^{-1}$)	1.0E+2	10.0E+1	2.0E+2
Hole mobility ($cm^2V^{-1}\ s^{-1}$)	2.5E+1	1.0E-1	8.0E+1
Shallow uniform donor density ND (cm^{-3})	Varied	0	0
Shallow uniform acceptor density NA (cm^{-3})	0	Varied	Varied

Table 2 Parameters of front and back contacts

Parameters	Front contact	Back contact
Surface recombination velocity of electrons (cm/s)	1.00E+7	1.00E+5
Surface recombination velocity of holes (cm/s)	1.00E+5	1.00E+7
Metalwork function (eV)	4.6039	5.8973
Majority carrier barrier height relative to E_f (eV)	0.0539	0.1527
Majority carrier barrier height relative to E_V (eV)	0.0000	0.0000

3 Methods

The simulator program SCAPS-1D has been used to perform the simulation of photovoltaic characteristic J-V and QE of the thin films n-ZnO/p-CuO and n-ZnO/p-Cu_2O solar cells. These characteristics allowed the calculation of the most important parameter such as open circuit voltage (Voc), short-circuit current (Jsc), fill factor (FF), and efficiency (eta), which were analyzed later. Simulations have been realized under standard illumination (AM 1.5 G, 100 MW.cm^{-2}, 300 K). The values of parameters of different materials have been taken from the literature and we have played on some of them to see their influence on the performance of the solar cell. The values shown in Table 1 are unchanged. We have inserted them into the program as such. On the other hand, the parameters whose influence we want to study have values that vary. For a variation of the values of one parameter, the other `parameters have a fixed value (the ideal value if found).Table 1 below shows the parameters of different materials.

The influence of the layers' thickness of different materials was analyzed as well as the influence of their bandgap. Additionally, the influence of the ND of ZnO and the influence of the NA of CuO and Cu_2O were also evaluated. Finally, we have used the best data to do the simulation for our cells. In Table 2 below, we have put the parameters for the front and back contact of the solar cell. This parameter has been taken in the simulation program.

Figure 1 below shows the structure of the two solar cells n-ZnO/p-CuO and n-ZnO/p-Cu_2O.

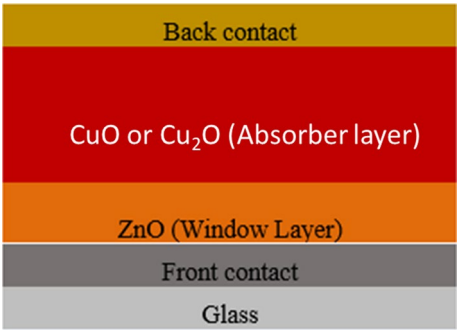

Fig. 1 Structure of the solar cell

4 Results and discussions

4.1 Influence of layers thickness

To determine the best ZnO layer thickness as a window layer in the different ZnO/CuO and ZnO/Cu_2O solar cells, the parameters Voc, Jsc, FF, and eta were constructed and depicted in Fig. 2 below. The smaller the thickness of the layer, the more the series resistance of the PV device is minimized (Sawicka-Chudy et al. 2019). The thickness varied from 50

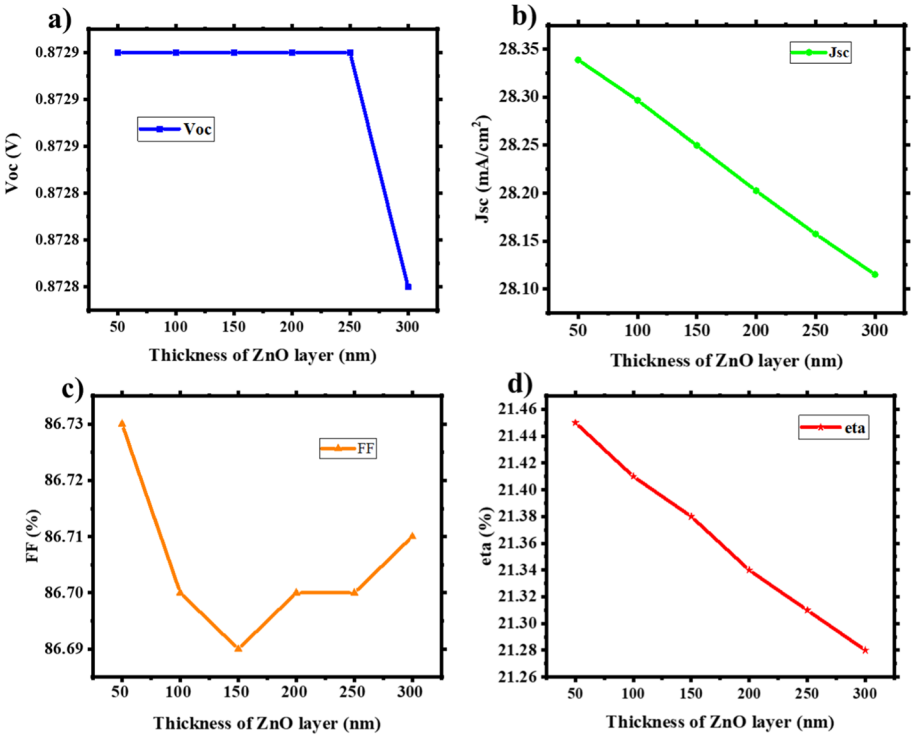

Fig. 2 Influence of ZnO thickness on the cell parameters

to 300 nm in the step of 50 nm. The bandgap and the shallow uniform donor density were kept as constants of 3.2 eV, 10^{17} cm^{-3}, respectively. Moreover, the parameters such as the thickness, the bandgap, and the shallow uniform acceptor of the CuO absorber layer were kept also as constants of 6000 nm, 1.51 eV, 10^{16} cm^{-3} respectively. The Voc depicted in a) was constant from 50 to 250 nm and decreases strongly. The other parameters decrease as increasing in the ZnO thickness. From these parameters, the optimal thickness of ZnO is 50 nm.

The influence of CuO thickness on the cell parameters is depicted in Fig. 3 below. The thickness varied from 3000 to 8000 nm in steps of 1000 nm. The bandgap and the shallow uniform acceptor density were kept as constants of 1.51 eV, 10^{16} cm^{-3}, respectively. The thickness, the bandgap, and the ND of the ZnO window layer were kept also as constants of 50 nm, 3.2 eV, 10^{17} cm^{-3} respectively. The figure shows that all parameters (Voc, Jsc, FF, eta) increase as the CuO thickness increases. The curves increase slightly after 600 nm. Thus, the best-chosen thickness is 600 nm.

The influence of Cu_2O thickness on the cell parameters is depicted in Fig. 4 below. The thickness varied from 500 to 4000 nm in steps of 500 nm. Here the bandgap and the shallow uniform acceptor density were kept as constants of 2.2 eV, 10^{18} cm^{-3}, respectively. The same ZnO parameters previously used were used. Among the curves below, only fill factor in c) decreases with the thickness increasing. Other curves increase as increasing in the Cu_2O thickness. The Jsc (Fig. 4b) and eta (Fig. 4d) increase strongly until 2000 nm

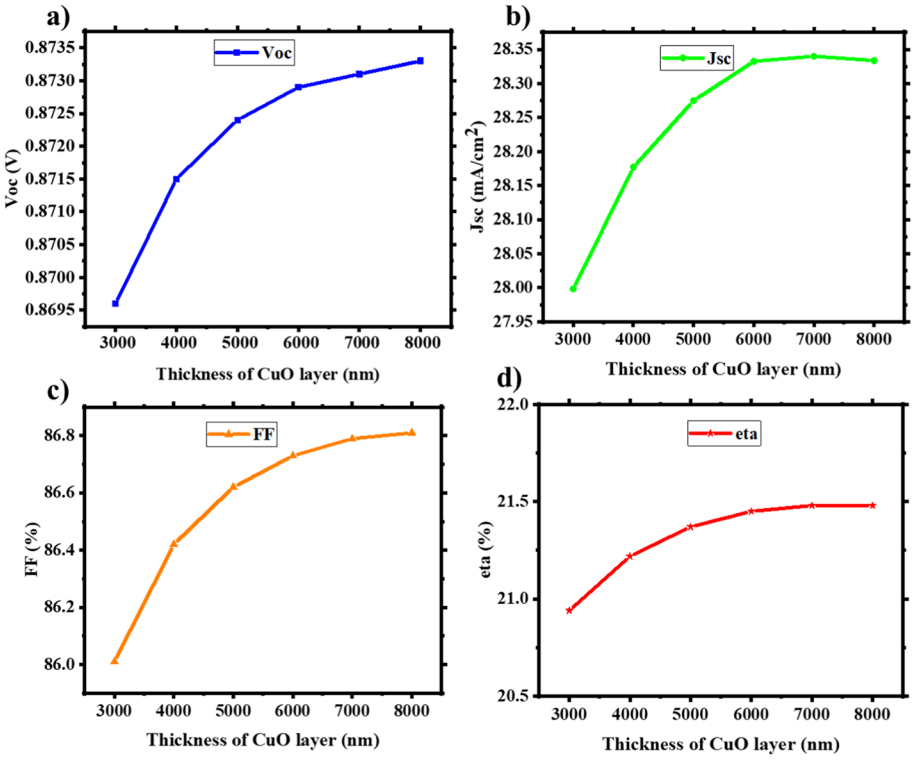

Fig. 3 Influence of CuO thickness on the cell parameters

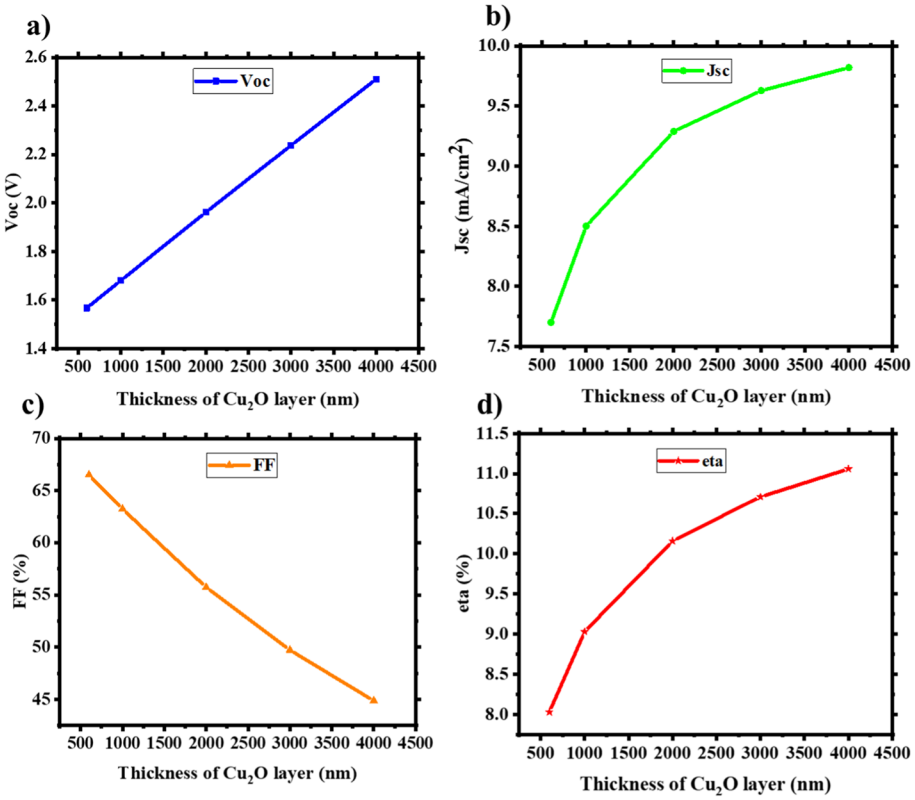

Fig. 4 Influence of Cu_2O thickness on the solar cell parameters

and increase slightly after this. The Voc (Fig. 4a) shows that a big thickness can be used to have good results, but the fill factor (Fig. 4c) will be small. From these different curves, 2000 nm was used as the Cu_2O thickness in this simulation.

4.2 Influence of bandgap

To determine the best bandgap of the ZnO layer, the bandgap varied from 2.2 to 3.3 eV and the different curves below were constructed in Fig. 5. The different parameters like the thickness of ZnO and CuO found previously were used as well as the other parameters of ZnO and CuO used previously. All curves below increase as the increase in ZnO bandgap. This increase is weak after 3.2 eV. Thus, 3.2 eV was used as the best bandgap of ZnO. It is possible to use 3.3 eV, but there won't be a big influence.

The influence of CuO bandgap on cell parameters is illustrated in Fig. 6 below.The bandgap was varied, and the other parameters used previously or found were kept constant. Unlike the values of Voc (Fig. 6a) and fill factor (Fig. 6c), the values of the Jsc (Fig. 6b) and the ete (Fig. 6d) decrease with the CuO bandgap increasing. As 1.5 eV has good results in each case, it was used as the CuO bandgap.

The influence of Cu_2O bandgap on the cell parameter is depicted in Fig. 7 below. ZnO and Cu_2O parameters used previously or found were kept constant, and the bandgap of

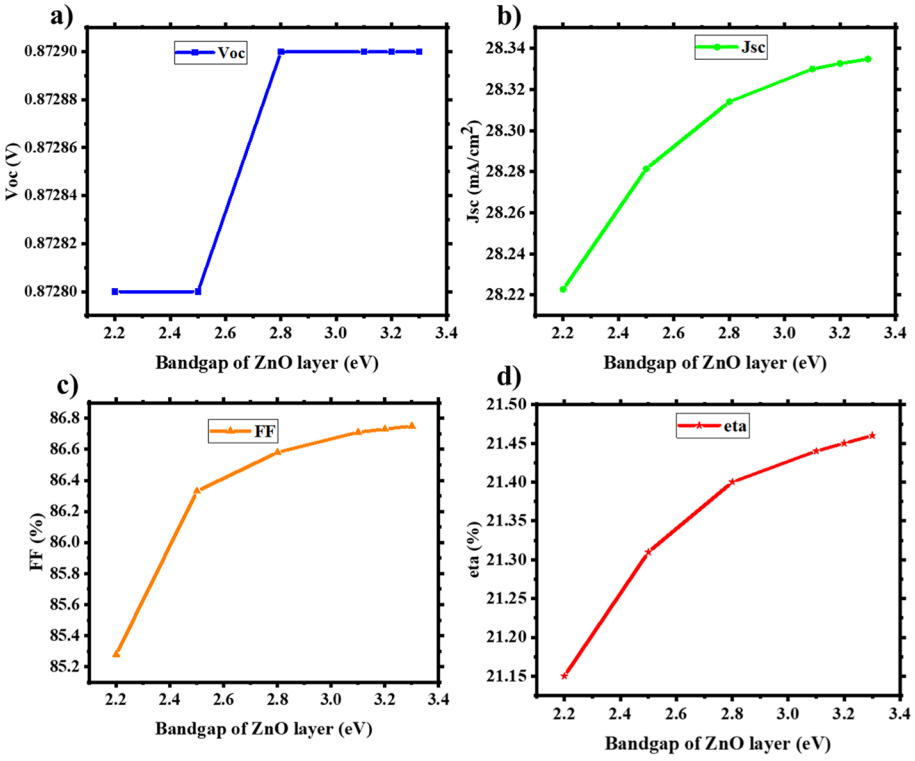

Fig. 5 Influence of ZnO bandgap on the cell parameters

Cu_2O varied from 2 to 2.2 eV. Results show that only the Voc increased with the bandgap from 2.1 eV. According to the results, the best bandgap is 2 eV with an efficiency of 11.8 eV.

4.3 Influence of ND and NA

Here, the influence of the ND and NA on cell parameters is studied. The parameters of different oxides used previously or found were kept constant and ND or NA varied. Results of the influence of ZnO's ND on cell parameters are in Table 3 below. The Voc rest constant with the ND variation. The Jsc decreases slightly with the ND increasing whereas the FF increase. The efficiency (eta) increases as the increase of ZnO ND. But the efficiency is constant after 10^{17} cm^{-3}. In this case, 10^{17} cm^{-3} was used as the best shallow uniform donor density of ZnO.

Table 4 below shows the results of the influence of CuO shallow uniform acceptor density on cell parameters. Results are good until the value 10^{22} cm^{-3}. After this value, the fill factor is bad (28.33%). Thus, the value 10^{22} cm^{-3} has been chosen as the best value of CuO shallow uniform acceptor density with an efficiency of 31.40%.

Results of the influence of Cu_2O shallow uniform acceptor density on cell parameters are in Table 5 below. The Voc and eta increase with the NA increasing which is opposite for the Jsc and FF. Contrary to previous results, the Jsc is weak at about 15 mA/cm^2 of

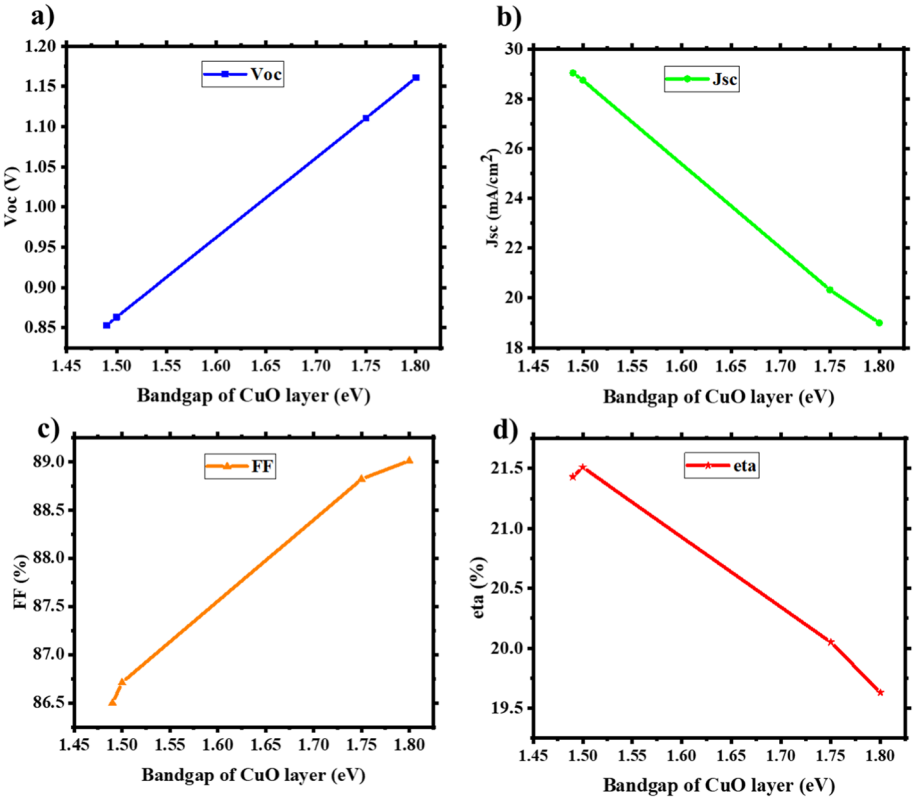

Fig. 6 Influence of CuO bandgap on the cell parameters

difference. Moreover, the efficiencies are weak compared to the efficiencies of the previous cell. According to the results, the fill factor is bad (FF = 39.93%) when NA is 10^{20} cm^{-3}. However, the different parameters have good results with a NA equal to 10^{19} cm^{-3}. Consequently, the value 10^{19} cm^{-3} has been chosen as the shallow uniform acceptor density of Cu_2O with an efficiency of 13.34% (Bouich et al. 2023; Bouazizi et al. 2023; Koné et al. 2023).

Figure 8 below summarizes the results of the two solar cells and allows to compare the different values. By comparison, the results of the solar cell-based-CuO are vastly superior to those of the solar cell-based-Cu_2O. For example, the efficiencies of solar cells n-ZnO/p-CuO and n-ZnO/p-Cu_2O were 31.40% and 13.34% respectively.

5 Conclusion

This work investigated the solar cell n-ZnO/p-CuO and n-ZnO/p-Cu_2O by using the solar cell simulator, SCAPS. The thickness, the bandgap, and the ND or NA of different layers were optimized by analyzing the results of Voc, Jsc, FF, and eta. After analyzing the ZnO film window layer, the optimized values of the thickness, the bandgap, and of the shallow uniform donor density are 50 nm, 3.2 eV, and 10^{17} cm^{-3} respectively. The values optimized

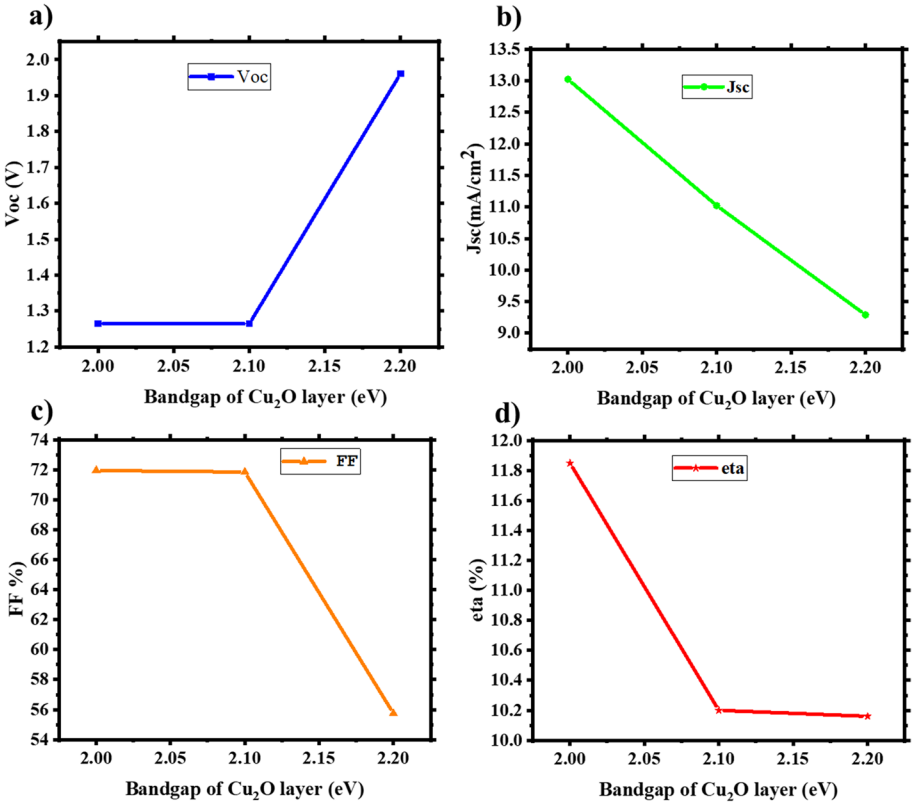

Fig. 7 Influence of Cu_2O bandgap on the cell parameters

Table 3 Influence of ZnO shallow uniform donor density on cell parameters

ND of ZnO (cm^{-3})	10^{15}	10^{16}	10^{17}	10^{18}
Voc (V)	0.8729	0.8729	0.8729	0.8729
Jsc (mA/cm^2)	28.3527	28.3542	28.3327	28.3017
FF (%)	86.49	86.63	86.73	86.82
Eta (%)	21.41	21.44	21.45	21.45

Table 4 Influence of CuO shallow uniform acceptor density on cell parameters

NA of CuO (cm^{-3})	10^{20}	10^{21}	10^{22}	10^{23}
Voc (V)	1.1347	1.1943	1.4666	4.1819
Jsc (mA/cm^2)	27.7954	27.7752	27.7755	27.7780
FF (%)	89.29	89.74	77.07	28.33
Eta (%)	28.16	29.77	31.40	32.92

Table 5 Influence of Cu_2O shallow uniform acceptor density on cell parameters

NA of Cu_2O (cm^{-3})	10^{18}	10^{19}	10^{20}
Voc (V)	1.2646	1.4295	2.8599
Jsc (mA/cm^2)	13.0250	12.9790	12.9698
FF (%)	71.96	71.90	39.93
Eta (%)	11.85	13.34	14.81

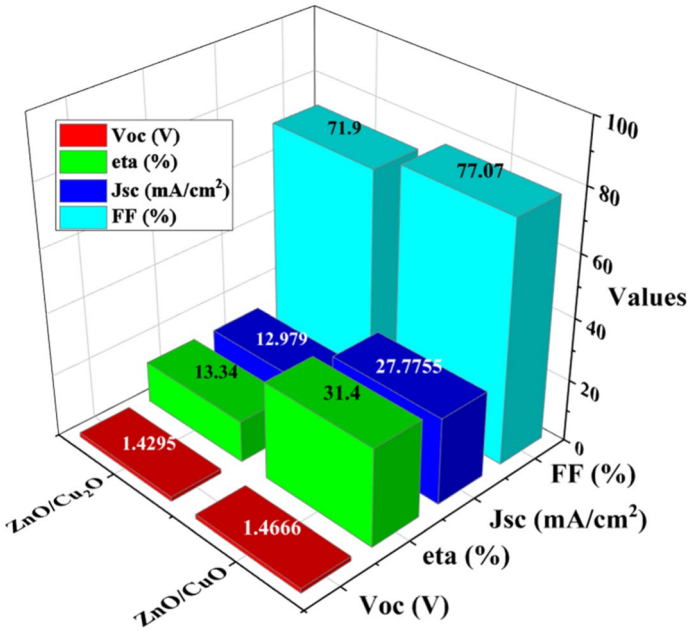

Fig. 8 Summary and comparison of the results of the two solar cells

for the thickness, the bandgap, and the NA of the CuO absorber layer are 6000 nm, 1.5 eV, and 10^{22} cm^{-3} respectively. The values optimized of these parameters and in this order of Cu_2O are 2000 nm, 2.2 eV, and 10^{19} cm^{-3}. With these different values optimized, the solar cell n-ZnO/p-CuO and n-ZnO/p-Cu_2O were 31.40% and 13.34% respectively. Results of the solar cell based-CuO are vastly superior to those of the solar cell based-Cu_2O. It is therefore the best solar cell for converting solar energy into electricity.

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Declarations

Ethical approval Not applicable.

Conflict interest The authors declare that they have no conflict of interest.

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