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Performance Enhancement Strategy of Ultra-Thin CIGS Solar Cells

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Abstract: In this article, numerical modeling and simulation using SCAPS-1D software has been used to explore the performance of CIGS-based solar cells when some parameters are modified. Starting from a baseline model that rigorously reproduces the experimental results, the absorber properties such as defect density, band-gap and acceptor concentration have been investigated and the optimal values to obtain high-efficiency CIGS-base solar cells have been proposed. The optimal parameters obtained are used to develop a new ultra-thin CIGS cell architecture. The results suggest that the use of 1000 nm Electron Back Reflector (EBR) layer with 1.3 eV band-gap at the CIGS/Mo interface provides higher electrical parameters than standard cells and materials such as MoS₂, AgO, SnS, Cu₂Te, CdSnP₂, CuIn₅S₈, PbCuSbS₃ can be successful EBR in ultra-thin CIGS solar cells. This optimized structure provides a serious pathway toward the development of ultra-thin cells with performance close to the best CIGS cells with standard thicknesses.

Keywords: Cu(In, Ga)Se₂, Band-Gap, Defect Density, Electron Reflector

Introduction

Thin-film solar cells represent a considerable hope in PV solar cells. They are studied in various laboratories to achieve the best quality/price ratio. Among thin-film solar cells, CIGS-based solar cells are popular because of their impressive performance. The efficiency of this solar cell has changed rapidly in the recent years due to the maturity of manufacturing techniques. The benefits of alkaline treatment have been mastered, resulting in a record efficiency of 23.35% (Nakamura *et al.*, 2019). However, this industry is confronted with a serious problem that compromises its long-term sustainability. Indium and gallium, which are widely used in the manufacture of CIGS-based solar cells, are rare (Rockett, 2010). To overcome this problem, several alternatives are proposed. The replacement of indium and gallium by more abundant, inexpensive and more environment-friendly metals such as zinc and tin to form a CZTS-based solar cell. However, the best CZTS solar cells obtained from substitute metals have a record yield of 12.6% (Wang *et al.*, 2014) far from the performance of CIGS-based cells. Reducing the thickness of the CIGS absorber layer seems to be a viable option (Chen *et al.*, 2019). Indeed, the standard thickness of the absorber in CIGS solar cells is approximately 2.5 μm . If

this thickness can be reduced by 50% or even below 1 μm , the deposition time will be considerably reduced, as well as the raw material used (Chen *et al.*, 2019). However, reducing the thickness of the absorber is problematic. Even if the absorption coefficient of this alloy is high ($\approx 10^5 \text{ cm}^{-1}$), a reduction in absorption and therefore the photo-current is observed when the thickness is reduced (Gouillart *et al.*, 2019; Massiot *et al.*, 2020).

Several laboratories around the world have embarked on this challenge with almost mitigated results. The main problem is the decrease in the solar cell performance when the thickness of the absorber is reduced.

In this study, we used SCAPS-1D software to investigate the parameters responsible for electrical losses in ultra-thin CIGS solar cells. The influence of several properties of the absorber on the electrical parameters was analyzed as a function of thickness. The optimal parameters obtained will be used to propose a new ultra-thin CIGS architecture with performances similar to those of a standard structure.

Theoretical Approach

In this numerical simulation, we used SCAPS-1D software (Niemegeers and Burgelman, 1996). By

introducing the input parameters, SCAPS calculates the output parameters from three fundamental semiconductor equations: Poisson equation, electron and whole continuity equation. With appropriate boundary conditions, these equations are solved simultaneously to obtain at each point in the device the electronic potential, the hole quasi-Fermi level and electron quasi-Fermi level. From these state variables, the carrier concentrations, fields, currents, etc., can then be computed. The good agreement between the experimental results and those of the simulation justifies the choice of this software (Burgelman *et al.*, 2004). The structure of the solar cell used for the simulation is shown in Fig. 1a. It consists of Soda glass/Mo/CIGS/SDL/CdS/i-ZnO/ZnO:B. The SDL layer, generally referred to as the Surface Defect Layer (SDL), is formed on the absorber surface due to the diffusion of atoms at the CdS/absorber interface. To make our model relatively simple, interface defects have been omitted voluntarily to reduce the number of parameters that change the results. To make the model reasonably realistic, bulk mid-gap defect states are

introduced in each material as recombination parameters. CIGS layer absorption coefficient used in the simulation was calculated from the equation $\alpha = 4\pi k/\lambda$ and shown in Fig. 1b, where the optical constants k are extracted from references (Paulson *et al.*, 2003) and λ the wavelength. The absorption data used for CdS, i-ZnO and ZnO:B layer are from experimental files introduced in SCAPS software. The temperature of the cell is set at 300 K. The AM1.5 spectrum was used as the incident light radiation on the cell.

The parameters used for our simulation are summarized in Table 1. These data are largely obtained from experimental and theoretical results in the literature (Gloeckler *et al.*, 2003; Pettersson *et al.*, 2011; Ouédraogo *et al.*, 2014). To test the robustness of our model, the I-V characteristic obtained from the parameters of Table 1 was compared to the experimental one (Fig. 1c) from (Pettersson *et al.*, 2011). A good agreement is achieved between the experimental and theoretical I-V characteristic data. The equivalent band diagram is shown in Fig. 1d.

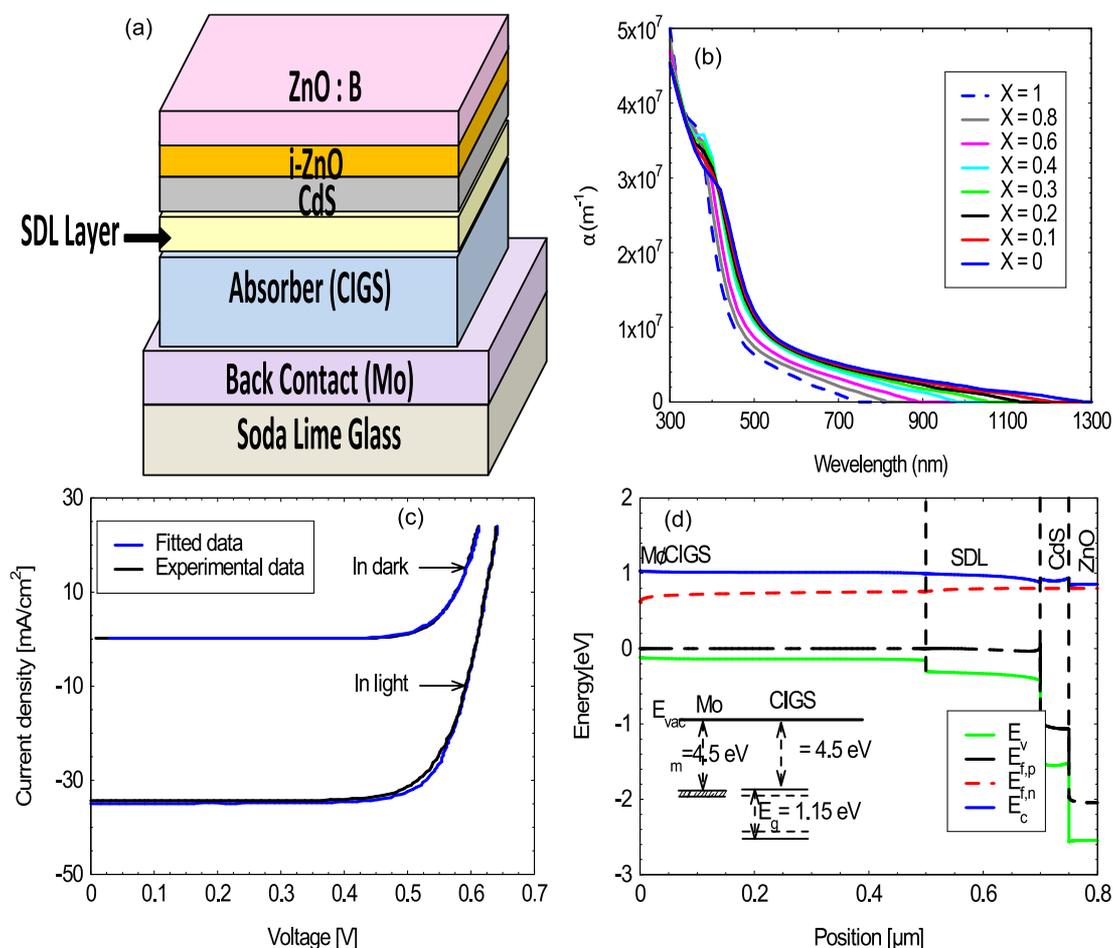


Fig. 1: (a) Solar cell structure used for simulation; (b) Absorption coefficients versus wavelength; (c) I-V characteristic compared to experimental results; (c, d) Equivalent energy band diagram of the solar cell under non-equilibrium conditions

Table 1: The solar cells simulation parameters used in SCAPS-1D

Parameters	CIGS	SDL	CdS	i-ZnO	ZnO:B
Layer properties					
Layer thickness (nm)	Variable	Variable	50	200	400
Layer band-gap: E_g (eV)	Variable	Variable	2.4	3.3	3.3
Electron affinity: χ (eV)	Variable	Variable	4.45	4.55	4.55
Dielectric relative permittivity: ϵ/ϵ_0	13.6	13.6	10	9	9
Conduction band effective density of states: N_c (cm ⁻³)	2.2*10 ¹⁸	2.2*10 ¹⁸	1.3*10 ¹⁸	3.1*10 ¹⁸	3*10 ¹⁸
Valence band effective density of state: N_v (cm ⁻³)	1.5*10 ¹⁹	1.5*10 ¹⁹	9.1*10 ¹⁸	1.8*10 ¹⁹	1.8*10 ¹⁹
Electron thermal velocity: v_e (cm/s)	3.9*10 ⁷	3.9*10 ⁷	3.1*10 ⁷	2.4*10 ⁷	2.4*10 ⁷
Hole thermal velocity: v_h (cm/s)	1.4*10 ⁷	1.4*10 ⁷	1.6*10 ⁷	1.3*10 ⁷	1.3*10 ⁷
Electron mobility: μ_e (cm ² /Vs)	100	variable	72	100	100
Hole mobility: μ_h (cm ² /Vs)	12.5	1.25	20	31	31
Doping concentration (cm ⁻³)	Variable	Variable	5*10 ¹⁷	10 ¹⁷	10 ²⁰
Bulk defect properties					
Defect density and type: N (cm ⁻³)	Variable (D)	Variable (D)	5*10 ¹⁶ (A)	10 ¹⁶ (A)	10 ¹⁶ (A)
Electron capture cross section: σ_e (cm ²)	10 ⁻¹⁵	10 ⁻¹³	10 ⁻¹⁵	10 ⁻¹⁵	10 ⁻¹⁵
Hole capture cross section: σ_h (cm ²)	10 ⁻¹¹	10 ⁻¹⁵	5*10 ⁻¹³	5*10 ⁻¹³	5*10 ⁻¹³

Results and Discussion

Effect of Absorber Thickness

To reduce the absorber thickness, it is necessary to understand how the electrical parameters change as the thickness changes. In most cases, reducing the absorber thickness is accompanied by a reduction in the absorber quality (Han *et al.*, 2012). To consider the absorber quality, three scenarios were considered. In the first (high quality), the absorber bulk defect was significantly reduced and the effective charge carrier's lifetime is 10 times greater than the traditional lifetime in CIGS solar cells (Repins *et al.*, 2009). In the "reasonable quality" scenario, the defect density is introduced to obtain the average lifetime in CIGS solar cells. Finally, in the "poor quality" scenario, a large quantity of bulk defects has been introduced in the absorber. The effect on the electrical parameters in these 3 scenarios as function of the absorber thickness is shown in Fig. 2. As can be seen, V_{oc} (Fig. 2a) and J_{sc} (Fig. 2b) are more affected when the absorber thickness is reduced (ultra-thin layer less than 0.5 μm). This solar cell response can be attributed to a poor absorption of incident photons due to the thinning of the absorber layer and an increase in back contact recombination due to the increased proximity of the back interface for thin CIGS layers (Gouillart *et al.*, 2019; Massiot *et al.*, 2020). Below 0.5 μm , this decrease is significant and leads to low efficiency. However, the electrical performance of the device as a function of the thickness depends strongly on the absorber quality. Solar cell electrical performance is bad with high absorber bulk defect (poor quality) and ultra-thin absorbers. For high-quality absorbers, the reduction of recombination via defects leads to high performance due to the long lifetime of the photo-generated carriers.

Effect of Acceptor Density and Absorber Quality

The acceptor density in the absorber is one of the parameters that can affect the performance of solar cells

(Ruckh *et al.*, 1996). However, doping control is recommended to optimize the performance of the device since, at high quantities, they affect the absorber's quality and therefore the lifetime of the charge carriers (Ouédraogo *et al.*, 2013). Figure 3 shows the impact of varying hole density (equivalent to the acceptor density) on the electrical parameters of our solar cell model.

V_{oc} increases significantly with the increase of the acceptor density (Fig. 3a). For acceptor density lower than 10¹⁴ cm⁻³, the absorber quality has no remarkable effect on V_{oc} but leads to low values of V_{oc} . However, the absorber quality becomes crucial to the V_{oc} when associated with high acceptor concentration.

When the acceptor density is less than 10¹⁴ cm⁻³, J_{sc} is more dependent on the absorber quality than the acceptor concentration. This means that, for moderate doping (small values of hole density), the quality of the absorber is a crucial factor on J_{sc} . A high quality absorber leads to high J_{sc} thanks to the reduction of absorber bulk recombination. For high acceptor concentrations (>10¹⁴ cm⁻³), J_{sc} decreases abruptly.

The FF (Fig. 3c) and conversion efficiency (Fig. 3d) increase with absorber doping but depend on the absorber quality. For poor quality absorbers with high hole density (>10¹⁶ cm⁻³), the performance of the cell is reduced. However, high conversion efficiency is achieved when a high-quality solar cell is associated with high doping (> 10¹⁶ cm⁻³). To increase the acceptor density, many experimental works have shown the benefit of alkaline treatment during the deposition of the CIGS absorber, which reduces the conversion efficiency deficit compared to the theoretical prediction due to the increase of acceptor concentration (Nakamura *et al.*, 2019). It appears that to obtain the beneficial effects of high acceptor density on the efficiency, it is crucial to have experimental conditions that allow the deposition of high-quality cells, which is consistent with the results obtained on the record cells (Nakamura *et al.*, 2019).

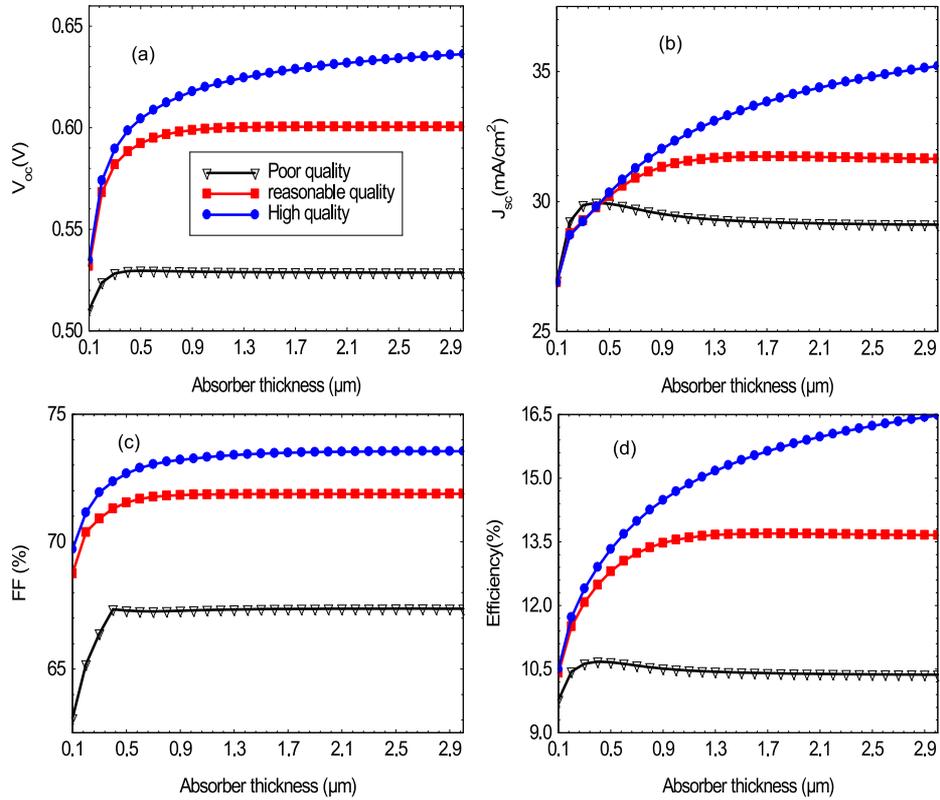


Fig. 2: Effect of absorber thickness and quality on electrical parameters: (a) V_{oc} , (b) J_{sc} , (c) FF and (d) conversion efficiency

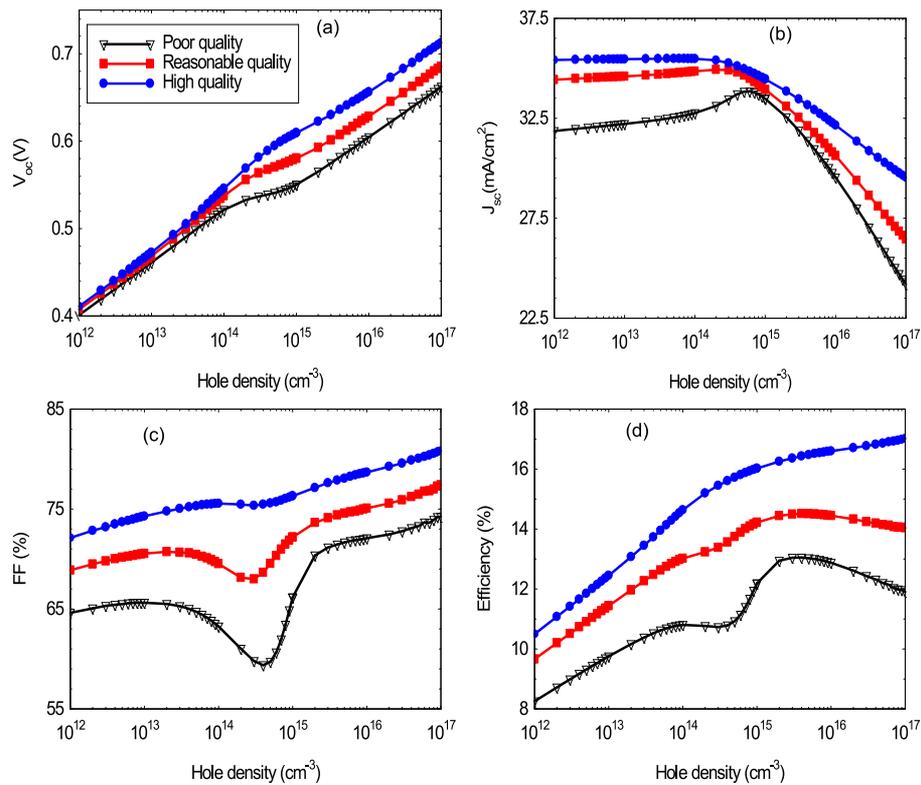


Fig. 3: Influence in the increase of hole density on the electrical parameters (J_{sc} , V_{oc} , FF, η) as a function of the absorber quality

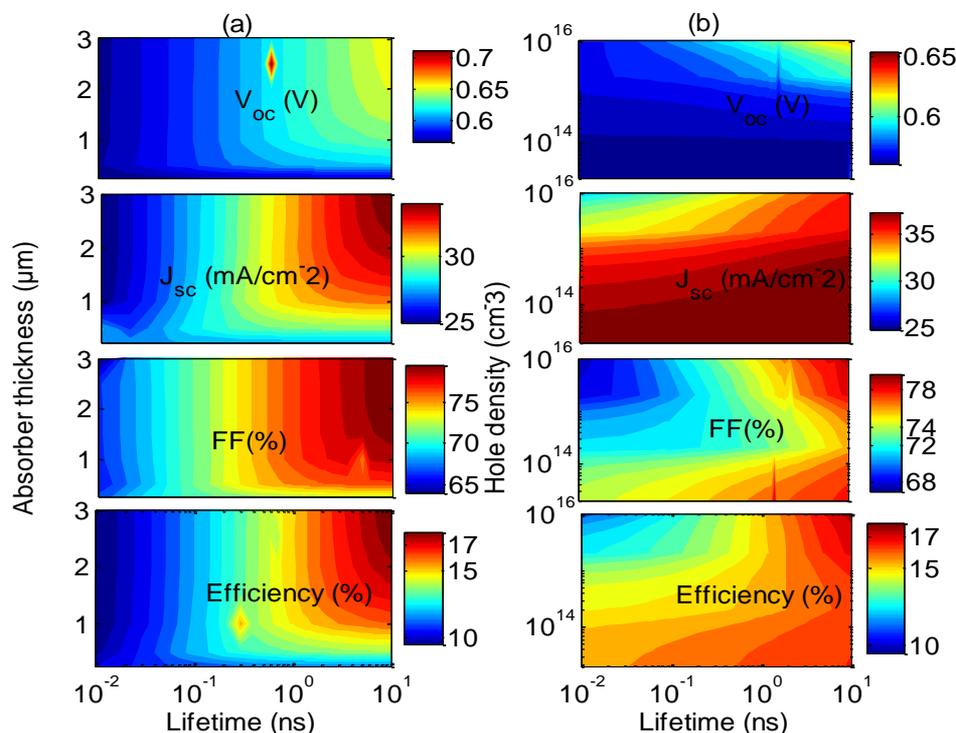


Fig. 4: Calculated impact of (a) absorber layer thickness and lifetime; (b) hole density and lifetime on the electrical parameters

The absorber quality affects the photo-generated charge carriers lifetime and therefore the performance of the cell. Figure 4 highlight how charge carriers lifetime impacts the solar cell electrical parameters when the thickness and hole concentration in the absorber are used as a variable. In Fig. 4a, the absorber thickness and carrier lifetime are varying. For short lifetimes ($< 10^{-1}$ ns), the electrical parameters are negatively affected when the absorber thickness increases. Indeed, a short lifetime of photo-generated carriers will lead to an increase in recombination via defects, thus, reducing the efficiency of the solar cell. For high lifetime, the best electrical performance is obtained with absorber thickness greater than 1 μm . Even with high lifetimes, ultra-thin absorbers are more vulnerable to back-contact recombination, resulting in a low conversion efficiency. High conversion efficiency is achieved by combining a high lifetime (> 10 ns) with a thickness greater than 1 μm .

Figure 4b obtained by varying both hole density and carrier lifetime shows that high values of V_{oc} are reached when high hole concentration is associated with high lifetime, in agreement with the results of the references (Kanevce and Gessert, 2011; Kanevce *et al.*, 2017). Small values of J_{sc} and FF are achieved at high carrier concentrations and short lifetimes. This could be explained by the fact that increasing the whole density beyond a certain value (10^{14} cm^{-3} in our study) reduces the Space-Charge Region (SCR). The quantities of

photo-generated charge outside the SCR become important and must diffuse to the SCR to be collected. Combined with a short lifetime, these photo-generated carriers have a high probability to recombine before reaching the ZCR, which explains the low values of J_{sc} and FF. Finally, the best conversion efficiencies are obtained at a high carrier concentration and long lifetimes.

Effect of Ga-Content of the Absorber

The gallium content in the absorber layer is an important factor to improve the performance of CIGS based solar cells. The introduction of Ga into the absorber layer conduct to a widening of the band-gap from 1.02 to 1.67 eV i.e., from the gap of the CIS to CGS film (Lundberg *et al.*, 2005). The variation of Ga-content affects also CIGS properties, such as conduction band (Lundberg *et al.*, 2005), absorption coefficient (Alonso *et al.*, 2002; Paulson *et al.*, 2003), defect density (Hanna *et al.*, 2001; Heath *et al.*, 2002). Defect density in the absorber is highlighted as the factor limiting the performance of CIGS cells at high Ga concentrations (Hanna *et al.*, 2001; Heath *et al.*, 2002). Figure 5 shows the experimental and simulated Quantum Efficiency (QE) as a function of Ga-composition. The classical three-stage deposition process was used for the sample fabrication. The simulation was performed with SCAPS by computing the band-gap and electron affinity for a given value of Ga-concentration. The Defects densities (D_d) were adjusted to reproduce the experimental QE. As

shown in Fig. 5, the simulated and experimental results are in excellent agreement. Moreover, the defect density decreases to a minimum when the Ga concentration is around 0.3, which justifies the high efficiencies CIGS cells obtained at this Ga concentration (Huang, 2008). Beyond this concentration, the defect density increases. Inserted in Fig. 5d represents the defect density profile as a function of Ga-content with a comparison to the single-stage deposition process from reference (Hanna *et al.*, 2001).

The defect profile as a function of Ga-content is introduced into the simulation. Figure 6 shows variations in electrical parameters when the absorber band-gap and thickness are used as variables. The quality of the absorber is also shown as a function of the band-gap range. The absorber quality affects the diffusion length and therefore the absorber thickness is an important parameter in the simulation. The open circuit voltage (V_{oc}) increases with the absorber band-gap but not

proportionally. For high Ga-content, although E_g increases, V_{oc} remains relatively constant due to the increase in recombination rate of charge carriers, especially in the space charge region. V_{oc} reduction is related to the poor quality of the absorber. Nevertheless, it can be noted that the open circuit voltage is independent of the thickness of the absorber. The short-circuit current density (J_{sc}) decreases with the absorber band-gap. This decrease is especially important when the thickness of the absorber is small. This situation can be attributed to the reduction in the generation rate at the p-n junction due to the decrease in absorption and the increase in recombination at the rear contact when the thickness is significantly reduced. The efficiency of the solar cell as well as the Fill Factor (FF) increase with the band-gap and the best performance is obtained for $1.15\text{eV} < E_g < 1.35\text{ eV}$, which correspond to high quality absorbers. Above this value, the overall performance of the solar cell starts to fall.

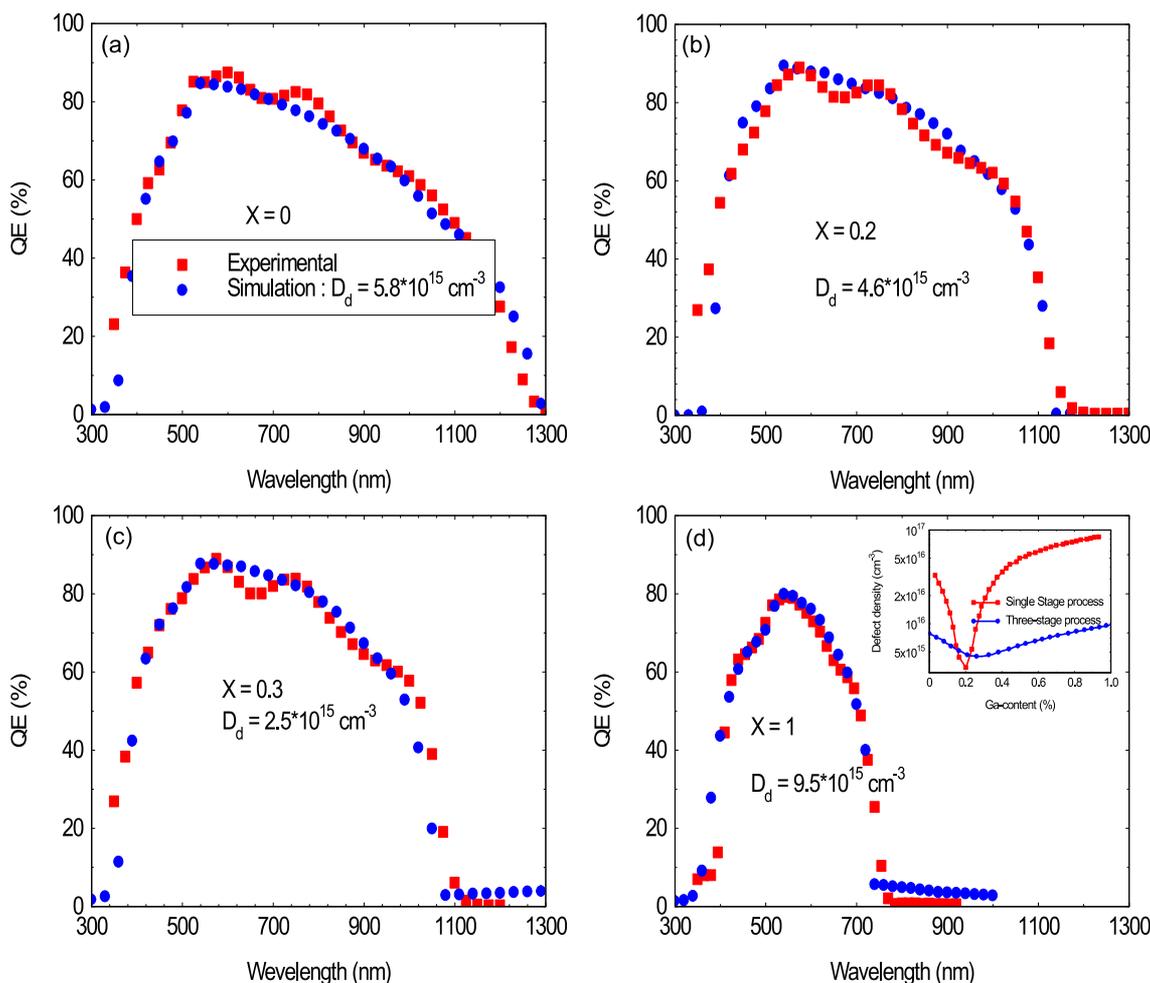


Fig. 5: Experimental quantification of Ga-content in the absorber on QE. The simulation was used to estimate defects concentration that reproduces the QE. Inserted in Fig. 5d represents the defect density profile as a function of Ga-content (Hanna *et al.*, 2001)

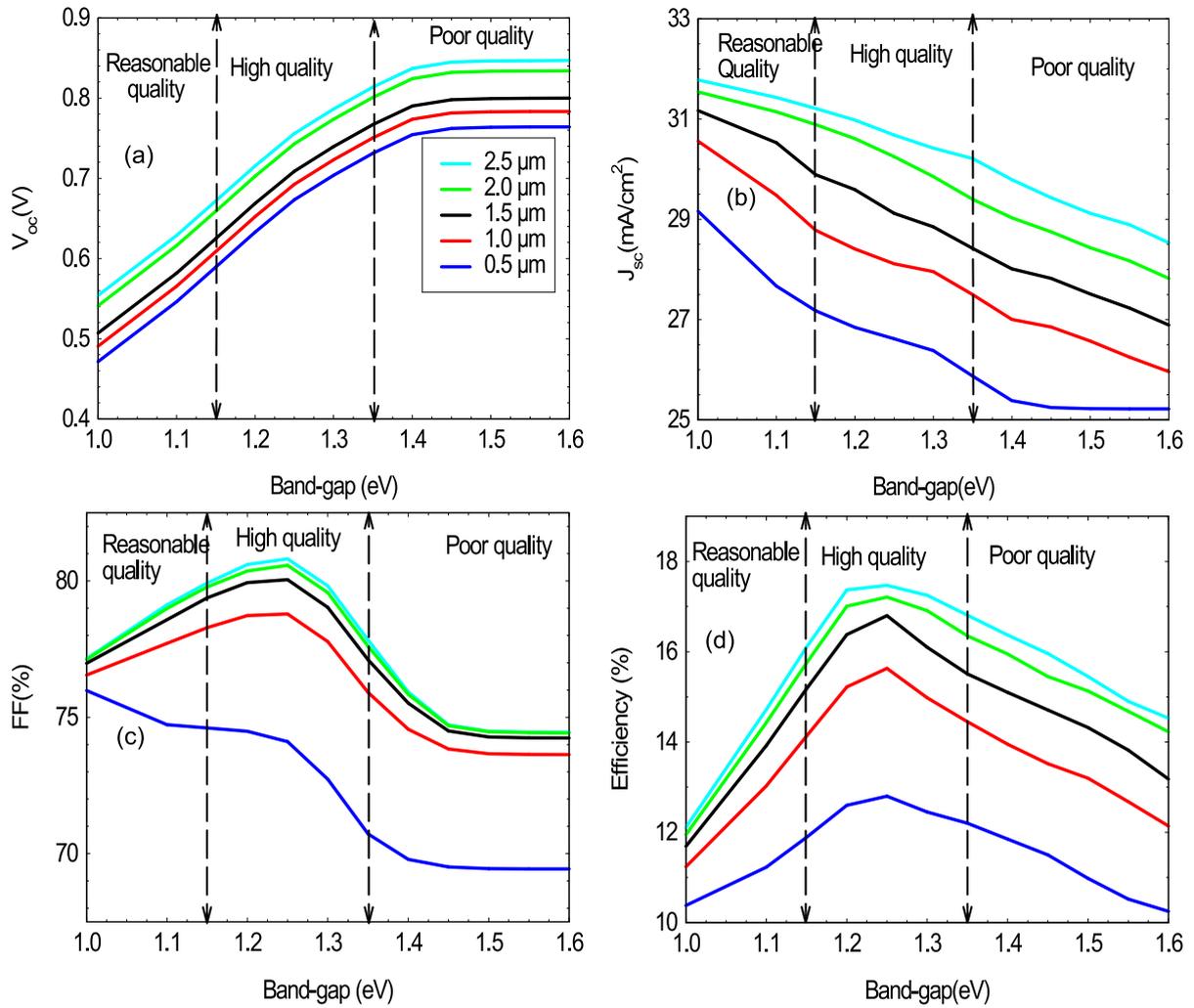


Fig. 6: Influence of absorber's band-gap and thickness on the electrical parameters (J_{sc} , V_{oc} , FF, Efficiency)

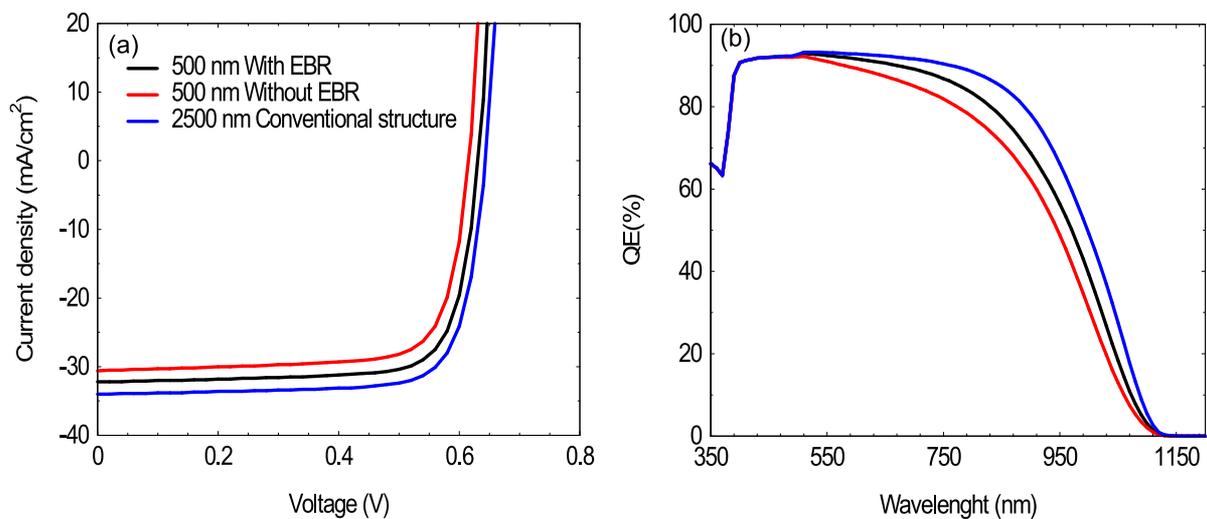


Fig. 7: (a) I-V characteristic and (b) quantum efficiency of an ultra-thin CIGS cell (500 nm) with and without EBR compared to the conventional structure (2500 nm)

Optimization of Ultra-Thin Absorbers

The optimal absorber properties found from the previous section are used to design a high conversion solar cell. Figure 7 shows the current-voltage characteristic and the quantum efficiency of CIGS solar cells with conventional larger thickness (2500 nm) and greatly reduced thickness (500 nm). Electrical parameters for these two configurations are shown in Table 2. When the thickness is considerably reduced compared to the conventional structure, high drop in J_{sc} is observed (Table 2). The current deficit between 500 and 2500 nm CIGS layer is 1.75 mA/cm² as a consequence of the reduction of absorption in the long wavelengths (Fig. 7b) and the increase in recombination at the back contact.

To improve J_{sc} in ultra-thin structures, one strategy is to introduce an electron reflector (commonly called EBR) at the interface between the CIGS and the Mo layers. When a thin EBR layer is introduced in 500 nm CIGS structure, an improvement of J_{sc} and efficiency is

observed (Table 2) through an improvement of the quantum efficiency (Fig. 7b).

Previous papers highlight that the important parameters for a best EBR layer are its band gap, thickness, acceptor density and electron affinity. Figure 8 shows the impact on J_{sc} and efficiency when EBR layer thickness and band-gap are taken as variables (Ouédraogo *et al.*, 2013). As can be seen in Fig. 8a, the increase in the EBR layer thickness leads to an increase in J_{sc} and the conversion efficiency of the ultra-thin CIGS cell due to the reduction of recombination rate at the CIGS/Mo interface combined with increased absorption. For ultra-thin absorbers, a large portion of the light passes through the absorber without being absorbed. The use of EBR layer allows the incident light to be reflected back to the absorber, increasing the electron-hole pair creation. A J_{sc} of 33.2 mA/cm² and an efficiency of 16.3% are obtained when the EBR layer thickness is 1000 nm.

Figure 8b shows the impact of the EBR band-gap (varying from 1.0 to 1.5 eV) on J_{sc} and conversion efficiency when its thickness is set to 1000 nm.

Table 2: Electrical parameters of an ultra-thin CIGS cell (500 nm) with and without EBR compared to conventional structure (2500 nm)

	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	Efficiency (%)
500 nm without EBR	0.6159	30.60	76.04	14.32
500 nm with EBR	0.6316	32.25	76.93	15.67
2500 nm	0.6435	34.00	77.28	16.91

Table 3: Electrical characteristics of an ultra-thin CIGS solar cell (500 nm thickness) with an optimized EBR layer at the CIGS/Mo interface compared to a conventional structure (2500 nm thickness)

	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	Efficiency (%)
500 nm with optimal EBR	0.7092	34.60	77.41	18.99
2500 nm CIGS absorber	0.6435	34.00	77.28	16.91

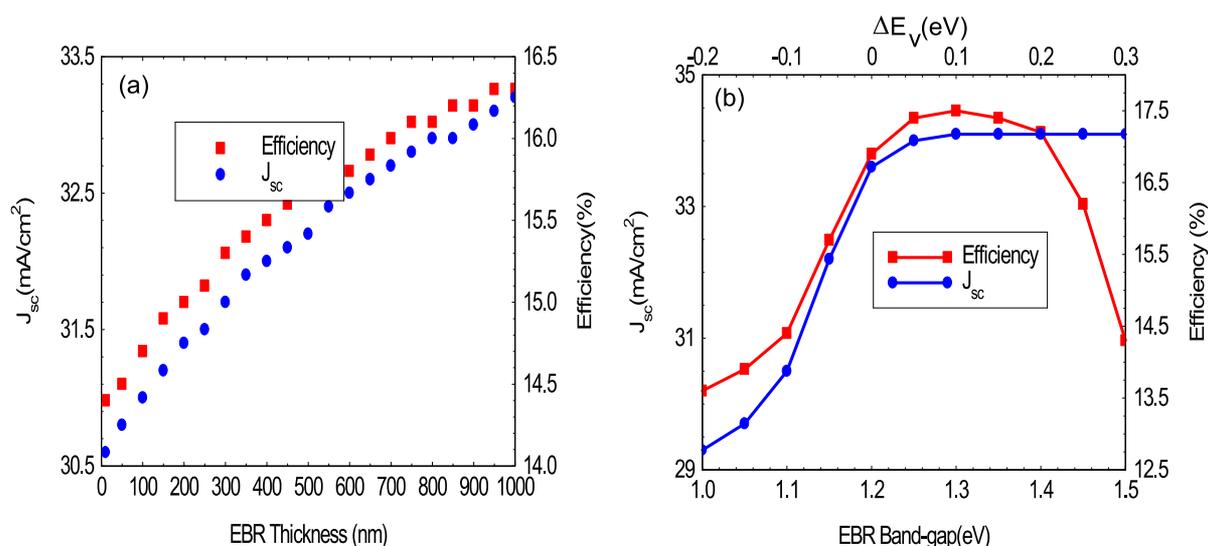


Fig. 8: Effect of EBR layer thickness (a) and band-gap (b) on J_{sc} and conversion efficiency

J_{sc} increases with the EBR layer band-gap and reaches a maximum value at 1.3 eV. Above this value J_{sc} seems to be insensitive to the increase in the EBR band-gap. The conversion efficiency profile is similar to J_{sc} for EBR band-gaps below 1.3 eV. However, more than 1.3 eV, the increase in the EBR band-gap is harmful to the performance of the solar cell, which is consistent with the contributions of other authors (Sharbati *et al.*, 2018) and confirms the accuracy of our model. This is due to a better alignment of the valence bands at the CIGS/EBR interface which allows a good collection of the photogenerated charges. However, above 1.3 eV, high barrier in the valence band is formed at the CIGS/EBR interface, blocking the collection of holes and leading to a drastic drop in conversion efficiency.

Table 3 shows the electrical characteristics of the ultra-thin (500 nm) CIGS cell when the optimal properties of the EBR layer are used in the simulation. The electrical characteristics of the classical structure (absorber thickness of 2500 nm without EBR) have been added for comparison. The results show that an ultra-thin (500 nm) CIGS cell with an optimized EBR layer provides high electrical characteristics compared to the thick cells. According to the EBR layer properties used in the simulation, materials such as MoS₂, AgO, SnS, Cu₂Te, CdSnP₂, CuIn₅S₈, PbCuSbS₃ can be successful EBR in ultra-thin CIGS solar cells.

Conclusion

In this study, we have explored CIGS-based solar cell and suggested pathways to improve its efficiency. The results of the simulation show that the absorber quality, band-gap, acceptor density and photo-generated charge lifetime are crucial parameters in the optimization of CIGS solar cells. After optimizing the absorber properties, a suitable strategy for producing an ultra-thin cell with comparable performance to conventional thick CIGS solar cells was proposed. The results suggest that the use of 1000 nm EBR layer with 1.3 eV band-gap provides high electrical parameters and materials such as MoS₂, AgO, SnS, Cu₂Te, CdSnP₂, CuIn₅S₈, PbCuSbS₃ can be successful EBR in ultra-thin CIGS solar cells. The results obtained in this study provide a pathway to improve and design ultra-thin cells with high conversion efficiency.

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Authors Contributions

Soumaïla Ouédraogo, Boureima Traoré and Marcel Bawindsom Kébré: Conceptualization, methodology, software, writing-original draft preparation.

Daouda Oubda, Adama Zongo and Issiaka Sankara: Data curation, methodology, software, original draft.

François Zougmore: Writing-reviewing and editing, supervision, validation, project administration.

Ethics

The Corresponding Author, declare that this manuscript is original, has not been published before. I can confirm that the manuscript has been read and approved by all named authors.

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