Scientific Research Publishing

Open Journal of Applied Sciences, 2025, 15(11), 3663-3672
https://www.scirp.org/journal/ojapps
ISSN Online: 2165-3925
ISSN Print: 2165-3917

# Numerical Simulation of the Dominate Recombination Mechanism in the Chalcopyrite $Cu(In,Ga)Se_2$ Thin Film Solar Cell

**Daouda Oubda*, Alain Diasso, Boureima Ouédraogo, Sayouba Kabré, Marcel Bawindsom Kébré, Soumaïla Ouédraogo, Boureima Traoré, Adama Zongo, Issaka Sankara, Pindéwindé Sawadogo, Amidou Barry, Boureima Sawadogo, François Zougmoré**

LA.M.E (Laboratory of Materials and Environment), UFR-SEA (Training and Research Unit in Exact and Applied Sciences), Doctoral School of Sciences and Technologies, Joseph KI-ZERBO University, Ouagadougou, Burkina Faso
Email: daoudaoubd@gmail.com

**How to cite this paper:** Oubda, D., Diasso, A., Ouédraogo, B., Kabré, S., Kébré, M.B., Ouédraogo, S., Traoré, B., Zongo, A., Sankara, I., Sawadogo, P., Barry, A., Sawadogo, B. and Zougmoré, F. (2025) Numerical Simulation of the Dominate Recombination Mechanism in the Chalcopyrite $Cu(In,Ga)Se_2$ Thin Film Solar Cell. *Open Journal of Applied Sciences*, **15**, 3663-3672.
https://doi.org/10.4236/ojapps.2025.1511238

**Received:** September 27, 2025
**Accepted:** November 18, 2025
**Published:** November 21, 2025



## Abstract

In a context marked by the increased use of energy which powers all the activities that make up economic life. The search for short and long term solutions involves improving the performance of renewable energy production systems in general and solar photovoltaic (PV) energy in particular. In the field of solar PV, research is underway to meet these requirements. Therefore, in this paper we present a numerical characterization of chalcopyrite copper-indium-gallium-diselenide thin film solar cells using one dimensional simulation program. Charge carrier recombinations play a major role in CIGS-based solar cells, as a result, the reduction in the lifespan of the charge carriers in the volume of the absorber leads to their recombination and explains the drop in performance. On the other hand, $V_{OC}$ increases with the increase in the gap and $J_{SC}$ decreases. If the energy of the conduction band discontinuity is equal to 0.1 eV, *FF* and $\eta$ decrease, $J_{SC}$ decreases suddenly for $\Delta E_C = 0.4$ eV. From our study, it appears obvious that as the surface recombination speed increases, the electrical performance of the solar cell decreases. When the interface recombination speed is $10^3$ cm/s, for $0.3 \le \Delta E_C \le 0.6$ eV, we note a significant decrease in efficiency with a value of 20.9%. The activation energy, denoted $E_a$, is a phenomenological parameter used to locate the place of predominance of SRH type recombination mechanisms in the CIGS solar cell. The study shows through the $J-V$ characteristic, a significant loss of the $J_{SC}$ by SRH recombination and confirm its domination. The consequences are therefore important, when the lifetime of the electron-hole pairs is at its basic value ( $\tau_{Vb} = 2\mu_s$ ), for $0.1 \le \Delta E_C \le 0.55\ \text{eV}$ , we note a reduction of 21.6% electrical conversion efficiency. The activation energy of a value of around 1.3 eV greater than the gap of the absorber ( $E_g = 1.2\ \text{eV}$ ) attest that SRH recombinations predominate inside the SCR.

**Keywords**

Numerical Simulation, Thin Film Solar Cell, Dominate Recombination Mechanism, Shockley-Read-Hall Recombination, Activation Energy

## 1. Introduction

Photovoltaic solar cells in general and in particular thin-film chalcopyrite solar cells based on copper-indium-gallium-selenium ($Cu(In,Ga)Se_2$) are increasingly promising. The record yields obtained so far bear witness to this, in 2019 by Nakamura achieved a record yield of 23.35% for solar cells [1]. Flexible solar panel modules recorded a record 22.22% efficiency in 2022 by the Swiss Federal Laboratories for Materials Science and Technology (EMPA) [1]. A record yield with the use of a zinc sulfide (ZnS) buffer layer reached 23.54% [2]. The technology offers excellent performance, in part thanks to its low temperature coefficient of only −0.36%/˚C [1].

Despite record yields which continue to increase and above all increasingly greater stability, PV solar cells based on the so-called second-generation quaternary CIGS system still encounter certain difficulties which affect their proper functioning [3]. Among these difficulties, we note the recombination mechanisms which manifest themselves in different localities of the solar cell [4]-[6]. The recombination mechanisms are the most determining factors in the operation of the solar cell, a good control of these recombination mechanisms would allow the improvement of the electrical parameters and the obtaining of significant conversion efficiency.

In this paper, our objective is to determine the type of recombination, Auger, radiative or Shockley-Read-Hall (SRH) mechanism dominant in the $Cu(In,Ga)Se_2$ solar cell model. In addition, we seek to know in which part, buffer layer (CdS), space charge region (SCR), CIGS/Mo interfaces, CIGS/CdS or CdS/ZnO interface, this type of recombination mechanism affects the most performance of the solar cell.

In the remainder of our article, we present the structure of the solar cell, we also present the software for simulating the capacities of one-dimensional solar cells (SCAPS-1D) used for the numerical simulation. Using numerical simulation, we determine the most dominant recombination mechanism, then we show the impact of these recombinations on the performance of the CIGS-based solar cell, finally we identify its predominance area.

## 2. Materials and Methods

### 2.1. Structure and Operating Principle of the CIGS-Based Solar Cell

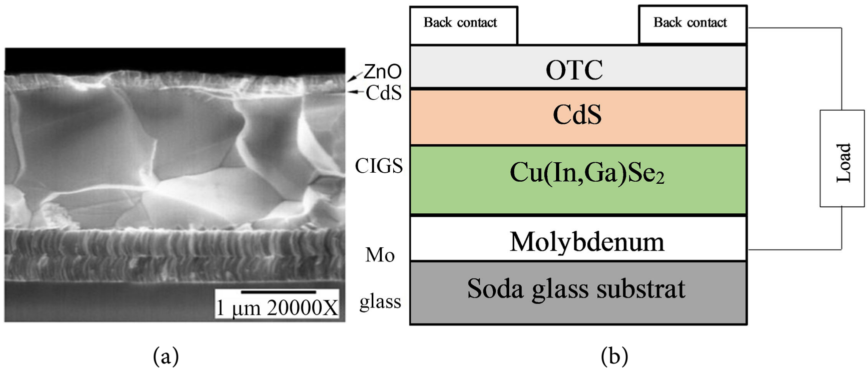


**Figure 1.** (a) Image of CIGS solar cell [7], (b) Structure of a CIGS-based solar cell [3].

**Figure 1** shows a photo of the sequence of layers of the model to be simulated. The different layers were experimentally deposited successfully at the National Renewable Energy Laboratory by K. Ramanathan [7]. We notice that the morphology of the layers differs depending on their physicochemical properties. The CIGS absorber which is the largest of the device occupies most of the surface of the solar cell [7] [8]. **Figure 1(b)** shows the structure of the CIGS-based solar cell with cadmium sulfide buffer layer that we extracted from the image (**Figure 1(a)**) [3]. We distinguish from bottom to top (**Figure 1(b)**): the substrate layer ($Na_2O_2$), the rear contact layer ($M_O$), the absorber layer (CIGS), the buffer layer (CdS), the conductive transparent oxide (ZnO) and the front contact layer (Ni/Al/Ni). The role and importance of each layer in the operation of the GIGS solar cell is described in detail in our previous work [4] [9] [10].

The study on the operating principle of this CIGS-based solar cell structure (**Figure 1(b)**) shows that photons with an energy $E_{ph} \prec 3.3\,\text{eV}$ pass through the ZnO layer. Those with an energy between 2.4 and 3.3 eV are absorbed in the CdS buffer layer. Once in the CIGS absorber, the incident photons are absorbed in the space charge region (SCR) [3] [4] [10]. The electron-hole pairs photogenerated in the SCR are separated by an internal electric field which respectively accelerates and propels the electrons at the front contact (Al/Ni) and the holes at the back contact (Mo) (**Figure 1(b)**) [4] [10]. It is very interesting to specify that the electric field comes from the presence of the heterogeneous p-n junction formed between the p-type CIGS layer and the n-type CdS layer. The electron-hole pairs which are collected at the front and rear contacts of the cell are delivered into the charge (**Figure 1(b)**) and give rise to a photocurrent generation.

### 2.2. One-Dimensional Solar Cell Capacity Simulation Software (SCAPS-1D)

Software developed by research teams is available in both free and paid versions. The most popular free software programs include: AFORS-HET (Automat for

Simulation of Heterojunction), ASA (Amorphous Semiconductor Analysis), AMPS-1D (Analysis of Microelectronic and Photonic Structures), and SCAPS-1D (Solar Cell Capacitance Simulator) [11].

SCAPS-1D is a one-dimensional numerical simulation software for Windows application, it is the work of focuses Marc Burgelman's team from the department of electronics and information systems (ELIS), at the University of Gent in Belgium. Its development is inspired by work on solar cells based on CdTe and Cu(In,Ga)$Se_2$ [12] [13]. The simulated results were in very good agreement with the measured results [14] [15] but, also with the results obtained with AMPS-1D [16]. SCAPS-1D on the most sensitive characteristics of the solar cell, namely: J-V, C-V, C-f and QE-$\lambda$ under illumination and darkness [1]. Taking into account defects that favor the recombination of charge carriers is effective with SCAPS-1D. The charge carrier recombination rate $R$ can be described by Equation (1) [3]:

$$R = \frac{1}{\tau_n} \frac{pn - n_i^2}{2n_i + p + n} \quad (1)$$

with $n$ the density of free carriers, $p$ concentration of holes, $n_i$ the density of intrinsic carriers, $\tau_n$ lifetime of electrons. The rate of generation of charge carriers due to optical excitation is given by Equation (2) [3]:

$$G(z) = -\frac{\mathrm{d}\Phi}{\mathrm{d}z} = \alpha_x \Phi(z_0) \exp\left(-\alpha_x (z - z_0)\right) \quad (2)$$

with $\Phi$ the photon flux density per unit area and time, $\alpha_x$ is the absorption coefficient, $\Phi(z_0)$ the flux density for an initial depth $z_0$, $z$ is the penetration depth of the flux.

Our study is based on a one-dimensional simulation, which has inherent limitations. Our model does not take into account lateral non-uniformities and the role of grain boundaries in polycrystalline films.

**Table 1** below shows the properties of the different layers of our PV solar cell model.

**Table 1.** Bases parameters of CIGS cell properties. $W$—thickness, $\varepsilon$—dielectric constant, $E_g$—band gap energy, $\Delta E_C$—conduction band offset, $\sigma_e$, $\sigma_h$—capture cross section electrons and holes, $\chi_e$—electron affinity, $\upsilon$—thermal velocity, $N_a$, $N_d$—shallow uniform acceptor and donor density. $d$—donnor, $a$—acceptor.

| Parameters | p-CIGS | n-CdS | n-OVC | i-ZnO | n-ZnO |
|---|---|---|---|---|---|
| $W$ [nm] | 1000 | 30 | 1 | 80 | 100 |
| $E_g$ [eV] | 1.2 | 2.4 | 1.45 | 3.4 | 3.3 |
| $\chi_e$ [eV] | 4.5 | 4.45 | 4.5 | 4.55 | 4.45 |
| $\varepsilon/\varepsilon_0$ | 13.6 | 10 | 13 | 9 | 9 |
| $N_c$ [$cm^{-3}$] | $2.2 \times 10^{18}$ | $2.2 \times 10^{18}$ | $2 \times 10^{18}$ | $4 \times 10^{18}$ | $2.2 \times 10^{18}$ |
| $N_v$ [$cm^{-3}$] | $1.8 \times 10^{19}$ | $1.8 \times 10^{19}$ | $2 \times 10^{19}$ | $3 \times 10^{19}$ | $1.8 \times 10^{19}$ |
| $v_e$ [cm/s] | $5 \times 10^6$ | $10^7$ | $5 \times 10^5$ | $10^7$ | $10^7$ |
| $v_h$ [cm/s] | $5 \times 10^6$ | $10^7$ | $5 \times 10^5$ | $10^7$ | $10^7$ |
| $\mu_e$ [$cm^2$/Vs] | $10^2$ | $10^2$ | 1 | 50 | $10^2$ |

Continued

| | | | | | |
|---|---|---|---|---|---|
| $\mu_h$ [cm²/Vs] | **25** | **25** | **1** | **20** | **25** |
| $N_a$ [cm$^{-3}$] | $2.5 \times 10^{16}$ [a] | - | $10^{13}$ [a] | - | - |
| $N_d$ [cm$^{-3}$] | - | $2.5 \times 10^{16}$ [d] | - | $5 \times 10^{17}$ [d] | $10^{18}$ [d] |
| $\sigma_e$ [cm$^2$] | $10^{-16}$ | $10^{-12}$ | $10^{-15}$ | $10^{-15}$ | $10^{-14}$ |
| $\sigma_h$ [cm$^2$] | $10^{-16}$ | $10^{-12}$ | $10^{-15}$ | $10^{-15}$ | $10^{-15}$ |
| $N_t$ [cm$^{-3}$] | $10^{15}$ [d] | $10^{16}$ [a] | $10^{15}$ [d] | $10^{14}$ [a] | $10^{13}$ [a] |

## 3. Results and Discussions

### 3.1. Dominant Recombination Mechanism

Charge carrier recombination plays a major role in CIGS-based solar cells. Controlling the different recombination mechanisms is very important for better performance of solar cells. The recombination of a charge carrier depends on its lifetime $\tau$, its mobility $\mu$, its diffusion length ($L$) and its recombination speed ($\upsilon_{th}$) [3]. There is radiative type, Auger type and Shockley Read Hall (SRH) type recombination mechanisms.

The simulation with SCAPS-1D allows us to obtain **Figure 2**, it highlights the effects of the different recombination mechanisms on the $J-V$ characteristic. Analysis of the results obtained in **Figure 2** shows a significant loss of current density by SRH type recombination. We deduce from these results that SRH type recombinations are dominant in the CIGS solar cell studied.

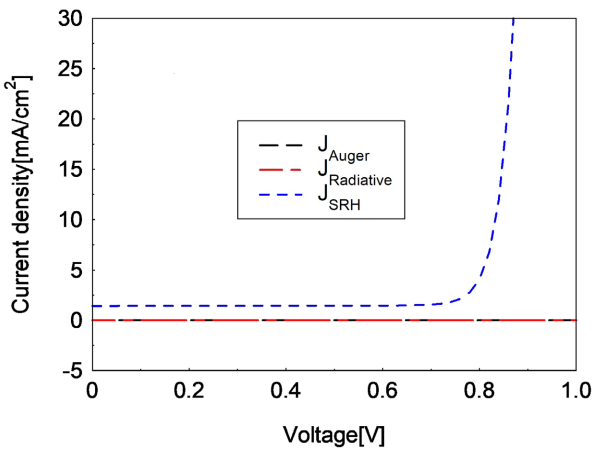


**Figure 2.** Recombination current density.

### 3.2. Impact of Volume Recombinations on Electrical Performance

Following the study which made it possible to determine the dominant type of recombination, we set ourselves in this part the objective of evaluating the impact of recombinations in volume and at layer interfaces on electrical performances.

The electrical performance of the CIGS-based solar cell decreases on the one hand with the reduction in the lifespan of the charge carriers (**Figure 3**). As a result, the reduction in the lifespan of the charge carriers in the volume of the absorber leads to their recombination and explains the drop in performance. On the other hand, $V_{OC}$ increases with the increase in the gap and $J_{SC}$ decreases (**Figure 3(a)** and **Figure 3(b)**). If the energy of the conduction band discontinuity is equal to 0.1 eV ( $\Delta E_C = 0.1\,\text{eV}$ ), $FF$ and $\eta$ decrease (**Figure 3(c)** and **Figure 3(d)**), $J_{SC}$ decreases suddenly for $\Delta E_C = 0.4\,\text{eV}$ (**Figure 3(b)**). These discontinuities correspond to energy barriers for the electrons photogenerated in the absorber. If the height of the barrier is greater than 0.4 eV, the photogenerated electrons cannot cross it, which explains the fall of $J_{SC}$. The consequences are therefore important, when the lifetime is at its base value ( $\tau_{Vb} = 2\mu_s$ ), for $0.1 \le \Delta E_C \le 0.55\,\text{eV}$, we note a reduction of 21.6% in conversion efficiency (**Figure 3(d)**).

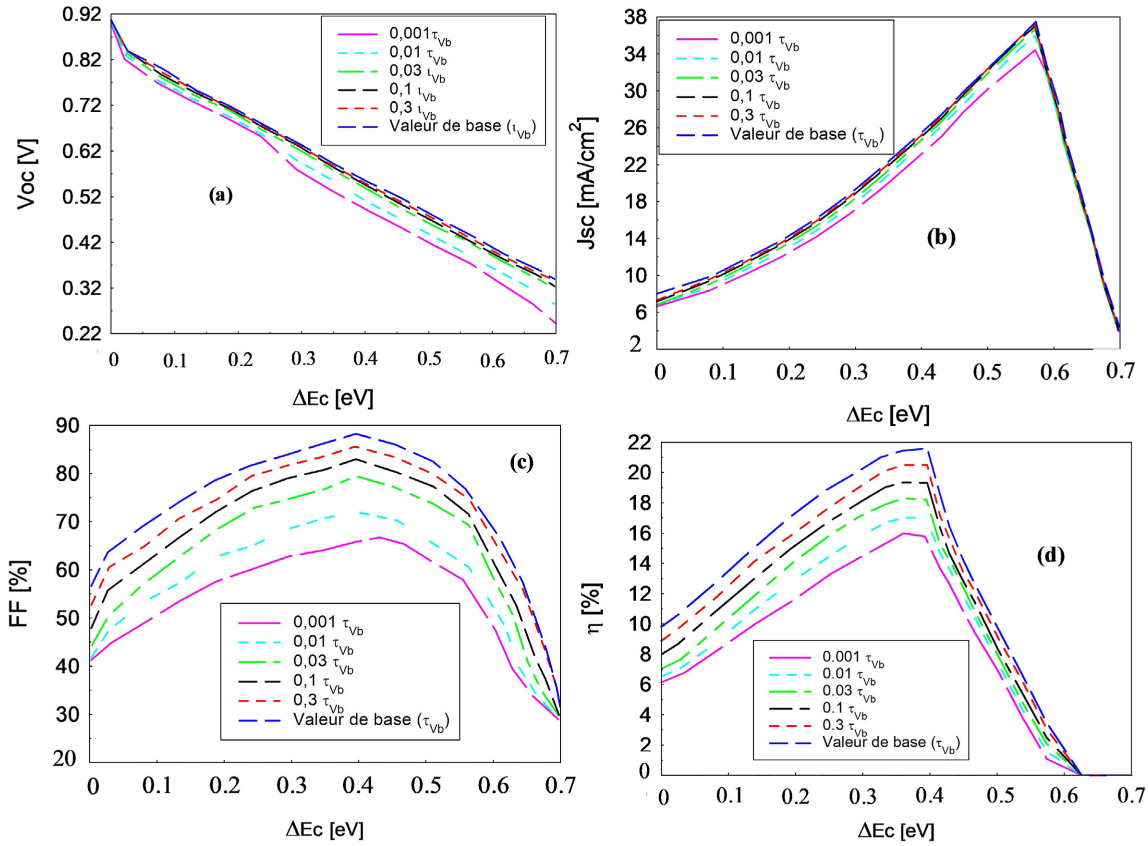


**Figure 3.** Effect of bulk recombination on electrical parameters.

## 3.3. Impact of Interface Recombinations on Electrical Performance

For the case of interface recombinations, they are characterized by the variation in the surface recombination speed ( $S$ ). From **Figure 4**, it appears obvious that as the surface recombination speed increases, the electrical performance of the solar cell decreases. Energy barriers appear for values $\Delta E_C = 0.1\,\text{eV}$ and 0.3 eV, which explains the significant reduction in the $J_{SC}$ (**Figure 4(a)**). Regarding interface recombinations, when the recombination speed is $10^3$ cm/s, for $0.3 \le \Delta E_C \le 0.6\,\text{eV}$, we note a significant decrease in efficiency with a value of

20.9% (**Figure 4(b)**).

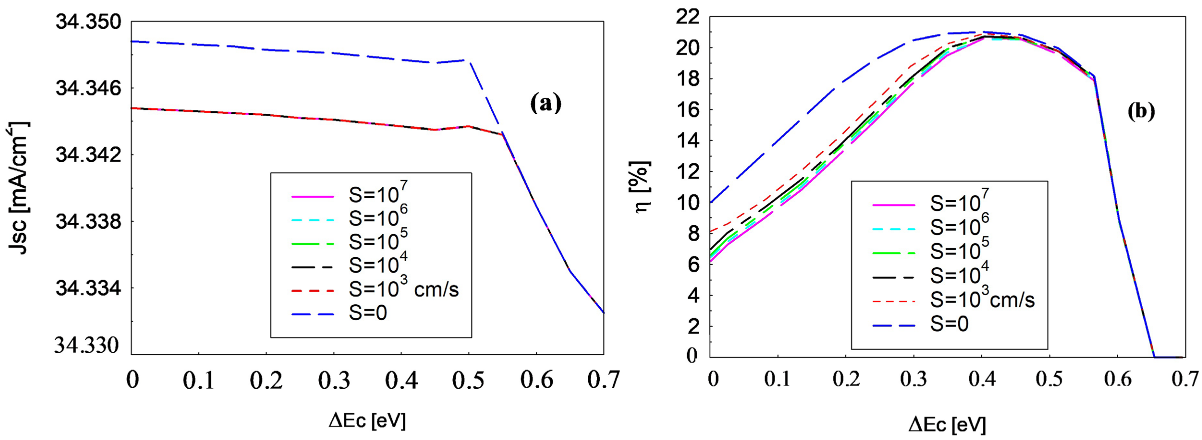


**Figure 4.** Effect of interface recombination on electrical parameters.

When two bandgap semiconductors Eg1 (CIGS) and Eg2 (CdS) are brought into contact, they exchange electrons to align their Fermi levels. Band alignment is important for solar cell performance because it strongly influences current transport across the junction. The energy difference between these two bandgaps determines the discontinuity of the conduction ($E_c$) and valence ($E_v$) bands at the interface of the two materials [7].

Two types of band discontinuity, namely a "peak" or a "cliff," can form between the CIGS absorber and the buffer layer [17]. A peak corresponds to a positive band discontinuity, meaning that the electron affinity of CIGS is greater than that of CdS, while a cliff corresponds to a negative band discontinuity. In this study, the band discontinuity in our model is a peak due to the fact that $\chi_{CIGS} \succ \chi_{CdS}$. A high energy peak at the CIGS/CdS interface blocks the flow of current in the solar PV cell.

## 3.4. Activation Energy

The activation energy, denoted $E_a$, is a phenomenological parameter used to locate the place of predominance of SRH type recombination mechanisms in the CIGS solar cell. In the literature, several methods exist for determining the recombination activation energy [4] [17]-[19].

The method that inspired us consists of plotting the $V_{OC}$ curve as a function of temperature and we use the following relation (Equation (3)):

$$V_{OC} \approx \frac{E_a}{q} - \frac{kT}{q}\ln\left(\frac{I_{ph}}{I_0}\right) \tag{3}$$

We graphically obtain the activation energy by extrapolating the curve up to the temperature of 0 K at the origin of the benchmark $\left(\frac{kT}{q}\ln\left(\frac{I_{ph}}{I_0}\right)\approx 0\right)$. The value of the $V_{OC}$ read corresponds to the value of the activation energy to a factor of $1/q$ ($V_{OC} = E_a/q$). We make the following hypotheses:

1) if the activation energy is lower than the absorber gap ($E_a \prec E_g$), the interface recombination mechanisms (CdS/CIGS, CIGS/Mo) are dominant;

2) if the activation energy is substantially equal to or greater than the gap of the absorber ($E_a \geq E_g$), the recombination mechanisms inside the SCR dominate.

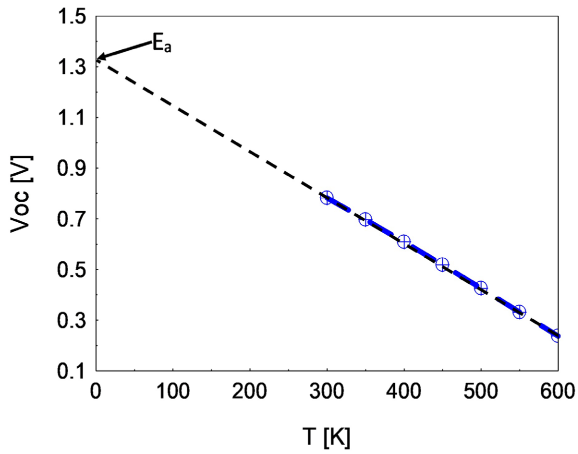


**Figure 5.** Method for determining activation energy.

From **Figure 5** obtained from the numerical simulation, we see that the activation energy of the model studied has a value of approximately 1.3 eV. This value is greater than the gap value of the absorber studied ($E_g = 1.2\text{ eV}$). In conclusion, the present model is affected more by SRH type recombinations in volume, more precisely inside the SCR.

## 4. Conclusions

In this paper, using the one-dimensional solar cell capacity simulation software (SCAPS-1D) we studied the $Cu(In,Ga)Se_2$ heterojunction solar cell by numerical simulation.

The study shows through the current-voltage density ($J-V$) characteristic a significant loss of short-circuit current density ($J_{SC}$) by SRH recombination. SRH recombinations, dominant in the CIGS solar cell, exert a considerable influence on these opto-electrical performances. The consequences are therefore important, when the lifetime of the electron-hole pairs is at its basic value ($\tau_{Vb} = 2\mu_s$), for $0.1 \leq \Delta E_C \leq 0.55\text{ eV}$, we note a reduction of 21.6% electrical conversion efficiency.

Our study allowed us to identify the predominance zone of these SRH recombinations, the activation energy of a value of around 1.3 eV greater than the gap of the absorber ($E_g = 1.2\text{ eV}$) attest that SRH recombinations predominate inside the space charge zone (SCR). Having determined the dominant recombination (SRH) mechanism in our CIGS-based solar cell model and its dominant recombination region (SCR), our next studies will focus on targeted defect passivation strategies during CIGS film growth.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

## References


[1] CIGS Layer Solar Panels: A Detailed Guide + the State of the Market (2023). https://fr.solarbuy.com

[2] Study by Numerical Simulation of a Solar Cell in CIGS. https://www.academia.edu

[3] Oubda, D. (2018) Characterization of Thin Film Solar Cell as Function of Buffer Layer Nature. Doctoral Thesis, University of Joseph KI-ZERBO.

[4] Oubda, D., Kebre, M.B., Ouédraogo, S., Zougmoré, F., Ouattara, F. and Koalga, Z. (2018) Numerical Characterization of $Cu(In,Ga)Se_2$ Solar Cells Using Capacitance-Voltage and Capacitance-Frequency Characteristics. *International Journal of Progressive Sciences and Technologies*, **6**, 262-267.

[5] Darga, A., Mencaraglia, D., Djebbour, Z., Dubois, A.M., Chouffot, R., Serhan, J., *et al.* (2009) Comparative Study of $Cu(In,Ga)Se_2/(PVD)In_2S_3$ and $Cu(In,Ga)Se_2/(CBD)CdS$ Heterojunction Based Solar Cells by Admittance Spectroscopy, Current-Voltage and Spectral Response Measurements. *Thin Solid Films*, **517**, 2423-2426. https://doi.org/10.1016/j.tsf.2008.11.017

[6] Huang, C.-H. (2008) Effects of Ga Content on $Cu(In,Ga)Se_2$ Solar Cells Studied by Numerical Modeling. *Journal of Physics and Chemistry of Solids*, **69**, 330-334. https://doi.org/10.1016/j.jpcs.2007.07.093

[7] Gloeckler, M. (2005) Device Physics of $Cu(In,Ga)Se_2$ Thin-Film Solar Cells. Ph.D. Thesis, Colorado State University.

[8] Ribeaucourt, L. (2011) Electrodeposition and Selenization of Cu-In-Ga Alloys for the Synthesis of Thin $Cu(In,Ga)Se_2$ Films for Solar Cells. Ph.D. Thesis, Pierre and Marie Curie University.

[9] Zongo, A., Oubda, D., Ouédraogo, S., Kébré, M.B., Diasso, A., Sankara, I., *et al.* (2021) Optimization of $Mo/Cu(In,Ga)Se_2/CdS/ZnO$ Hetero-Junction Solar Cell Performance by Numerical Simulation with SCAPS-1D. *Journal of Materials Science and Engineering B*, **11**, 156-167. https://doi.org/10.17265/2161-6221/2021.10-12.004

[10] Oubda, D., Kebre, M.B., Zougmoré, F., Njomo, D. and Ouattara, F. (2015) Numerical Simulation of $Cu(In,Ga)Se_2$ Solar Cells Performances. *Journal of Energy and Power Engineering*, **9**, 1047-1055. https://doi.org/10.17265/1934-8975/2015.12.002

[11] Diouf, D. (2010) Silicon Photovoltaic Cells with Heterojunctions and an Interdigitated Structure on the Rear Face. Ph.D. Thesis, University of Paris Sud-11.

[12] Niemegeers, A., Burgelman, M., Herberholz, R., Rau, U., Hariskos, D. and Schock, H.-W. (1998) Model for Electronic Transport in $Cu(In,Ga)Se_2$ Solar Cells. *Progress in Photovoltaics: Research and Applications*, **6**, 407-421. https://doi.org/10.1002/(sici)1099-159x(199811/12)6:6<407::aid-pip230>3.0.co;2-u

[13] Khelifi, S. and Belghachi, A. (2004) The Role of the Window Layer in the Performance of a GaAs Solar Cell. *Journal of Renewable Energies*, **7**, 13-21. https://doi.org/10.54966/jreen.v7i1.861

[14] Niemegeers, A. and Burgelman, M. (1997) Effects of the Au/CdTe Back Contact on IV and CV Characteristics of Au/CdTe/CdS/TCO Solar Cells. *Journal of Applied Physics*, **81**, 2881-2886. https://doi.org/10.1063/1.363946

[15] Burgelman, M., Nollet, P. and Degrave, S. (2000) Modelling Polycrystalline Semiconductor Solar Cells. *Thin Solid Films*, **361-362**, 527-532.

https://doi.org/10.1016/s0040-6090(99)00825-1

[16] Yiming, L., Yun, S. and Angus, R. (2011) A New Simulation Software of Solar Cells—wxAMPS. *Solar Energy Materials & Solar Cells*, **98**, 124-128.

[17] Ouédraogo, S. (2016) Numerical Modeling of a Thin-Film Solar Cell Based on CIGS. PhD Thesis, Ouaga I University.

[18] Rusu, M., Eisele, W., Würz, R., Ennaoui, A., Lux-Steiner, M.C., Niesen, T.P., *et al.* (2003) Current Transport in ZnO/ZnS/Cu(In,Ga)(S,Se)$_2$ Solar Cell. *Journal of Physics and Chemistry of Solids*, **64**, 2037-2040. https://doi.org/10.1016/s0022-3697(03)00175-6

[19] Hultqvist, A. (2010) Cadmium Free Buffer Layer and the Influence of Their Material Properties on the Performance of Cu(In,Ga)Se$_2$ Solar Cells. Ph.D. Thesis, Uppsala Universitet.