

Original Research Paper

Bulk and Interface Configuration on the Performances of Perovskite Solar Cells

Sankara Issiaka, Soumaïla Ouédraogo, Daouda Oubda, Boureima Traoré,
Marcel Bawindsom Kébré, Adama Zongo and François Zougmore

Department de Physique, Laboratoire de Matériaux et Environnement (L.A.M.E) - UFR/SEA,
Université Joseph Ki-Zerbo, Ouagadougou, Burkina Faso

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Corresponding Author:

Sankara Issiaka

Department de Physique,

Laboratoire de Matériaux et

Environnement (L.A.M.E) -

UFR/SEA, Université Joseph

Ki-Zerbo, Ouagadougou,

Burkina Faso

Email: sankaraissaka1@gmail.com

Abstract: The ongoing search for energy conversion technologies that are more efficient, affordable, and sustainable than traditional solar cells have led researchers to look at other technologies. Among these technologies, perovskite-based solar cells seem increasingly credible, as they have the potential to achieve high energy conversion efficiencies that rival or even surpass those of silicon solar cells, which currently dominate the market. Despite this enormous potential, perovskite solar cells face several problems holding them back. For this study, we employed the SCAPS-1D software which is a simulation software developed at the University of Ghent in Belgium for conducting numerical simulations of a perovskite solar cell. The calculation methodology is the finite difference method using the transport, Poisson, and continuity equations with predefined boundary conditions. Through this simulation, we studied the influence of absorber thickness, lifetime, carrier diffusion length, and defect density on the overall behavior of the electrical parameters. The best performances are observed when the absorber thickness is equal to 0.5 μm and the defect density is less than 10^{16}cm^{-3} .

Keywords: Perovskite, Defect Density, Thickness, Solar Cell, Scaps-1d Software

Introduction

Perovskite-based solar cells are currently at the heart of research in the photovoltaic sector. Their optical and electronic properties are attracting a great deal of interest in solar energy and emerging technologies. Perovskites have long been considered rare and of little use. However, extensive research has revealed their incredible potential as semiconductor materials, paving the way for a new era in electronics and solar energy. Perovskite-based solar cells currently have energy conversion rates of around 23% for single junctions, however, significant performance improvements of over 30% are possible by exploiting tandem configurations such as perovskite-silicon, perovskite-CIGS (Boumami, 2022; Asma, 2022) and perovskite-perovskite (McMillon-Brown *et al.*, 2021). These advances could make them suitable for several applications. Despite their impressive properties, perovskite-based solar cells face problems of stability and durability. These problems are linked to a lack of in-depth knowledge of the intrinsic properties that govern the operation of the perovskite cell. This article aims to

highlight the role of certain properties of the perovskite layer on the overall behavior of the structure. Firstly, the influence of the thickness of the absorber is studied, followed by the lifetime and diffusion length of the carriers, and finally the density of defects at the interfaces on the electrical parameters of the perovskite solar cell. Controlling and mastering these parameters would be the key to improving and stabilizing the efficiency of perovskite cells.

Materials and Methods

Solar Cells Structure

Researchers have developed software for numerical simulations to develop high-efficiency, low-cost solar cells. These software packages offer different possibilities and limitations, but the basic equations remain the same. In this study, we used SCAPS-1D software. This one-dimensional numerical simulation software was developed at the Electronics and Information Systems (ELIS) laboratory at the University of Ghent in Belgium. SCAPS runs on Windows. It was set up to simulate the

electrical parameters of heterojunction solar cells. It was tested on CdTe and Cu (In, Ga) Se₂ solar cells by Burgelman *et al.* (2000). The simulated and measured results were very satisfactory (Burgelman *et al.*, 2004). Subsequently, many improvements were made to SCAPS so that it could be used to model perovskite solar cells. With SCAPS-1D, it is possible to simulate structures made up of a defined number of layers (up to 7 intermediate layers plus front and back contacts) (Minemoto and Murata, 2014b), with different doping profiles and with given donor or acceptor level energy distributions, in the volume and at the interfaces for an arbitrary light spectrum.

Figure 1 shows the structure of a perovskite-based solar cell. It consists of a glass substrate onto which FTO-doped tin oxide is deposited. Titanium dioxide is then deposited on the FTO. The TiO₂ is an electron transport layer (ETM). The active layer (PVK) consists of a perovskite material. To improve hole transport, a layer of spiro-OMeTAD (HTM) is deposited between the gold electrode and the active layer.

Fundamental Equations in Simulation Software

Several years of research into the physics of semiconductor-based devices have led to the development of mathematical models. These models are essentially based on the resolution of the Poisson equation and the continuity equations for electrons and holes.

Poisson's Equation

Poisson's equation relates variations in electrostatic potential to local charge densities.

It is given by:

$$\text{div} \epsilon \nabla \psi = -\rho \quad (1)$$

where, ψ represents the electrostatic potential, ϵ is the dielectric permittivity ($\epsilon = \epsilon_0 \cdot \epsilon_r$ with ϵ_0 is the permittivity of the vacuum and ϵ_r is the relative permittivity of the material), ρ is the volume density of the free charges.

Continuity Equations

Continuity equations illustrate the variations in electron and hole densities in response to transport, generation, and recombination mechanisms.

The continuity equations are given by:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \text{div} \vec{J}_n + G_n - R_n \quad (2)$$

$$\frac{\partial p}{\partial t} = \frac{1}{q} \text{div} \vec{J}_p + G_p - R_p \quad (3)$$

G_n and G_p are degeneration rates for electrons and holes; R_n and R_p are respectively the recombination rates of electrons and holes; J_n and J_p are the densities of electron currents and holes.

Results and Discussion

The results of the numerical simulation of a perovskite-based solar cell using the SCAPS-1D software allowed us to determine the influence of certain material parameters on the electrical characteristics, to obtain optimal values. These parameters include interfering fault densities at the interfaces, charge carrier lifetime, and absorber thickness. The optimal parameters obtained could be used to make perovskite-based solar cells with higher performance than conventional cells.

Influence of Absorber Thickness

The absorber is the key component in thin-film solar cells and a detailed study of its parameters is essential for designing a high-performance solar cell. In this section, we varied the absorber thickness from 0.03-2 μm to study the impact of absorber thickness on the electrical parameters J-V and QE. Figure (2a) shows the influence of thickness on the current-voltage characteristic. All electrical parameters are affected by ultra-thin thicknesses. Ultra-thin solar cells have a very thin active layer, which can lead to a high carrier density and an increased probability of charge recombination when passing through the active layer (Gopal *et al.*, 2023). Figure (2b) shows the Quantum Efficiency (QE) as a function of thickness. It can be seen that the quantum yield varies slightly for wavelengths between 300 and 400 nm for the different thicknesses. However, above 400 nm, it falls sharply for thicknesses between 0.03 and 0.05 μm . The quantum yield stabilizes for thicknesses between 0.5 and 2 μm at wavelengths above 450 nm. The best Quantum Efficiency (QE = 87%) is obtained with a thickness of 0.5 μm for a wavelength greater than 450 nm. The high efficiency observed for the 0.5 μm thickness can be attributed to the thicker absorber layer can capture more incident light, increasing the probability of generating electron and hole pairs (electrical charges) from the absorbed light. However, the thickness of the absorber needs to be adjusted to allow optimum absorption of light across the solar spectrum because perovskites have absorption properties that depend on the thickness of the material and inadequate thickness can lead to under- or over-use of certain wavelengths of light.

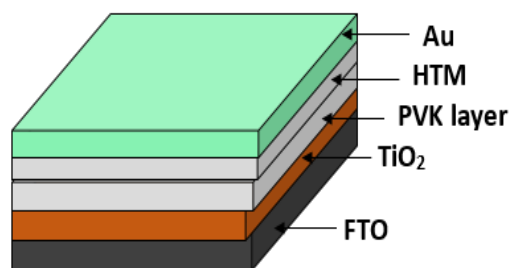


Fig. 1: Composition of a perovskite cell

Using the electrical parameters derived from the current-voltage characteristic (Fig. 2a), we study the influence of thickness on the electrical parameters as shown in Fig. 3. The open-circuit voltage (Fig. 3a) increases progressively with increasing thickness and decreases slightly after 2 μm . This results from an elevation in volume recombination. The short-circuit current density (Fig. 3b) increases with absorber thickness and saturates at around 24 mA/cm^2 when the thickness reaches 2 μm . This saturation is due to the reduction in the electric field in the absorber (Burgelman *et al.*, 2004). In addition, the thickness of the absorber layer can affect the amount of light that is absorbed by the cell. A layer that is too thin may not absorb enough light, while one that is too thick may reduce the amount of light that reaches the charge collection layers. Figure (3d) shows that the Form Factor (FF) reaches a maximum value of 80% for ultrathin layers and gradually decreases for thicknesses greater than 0.03 μm . This is because the form factor depends on the characteristic between the actual current-voltage curve of the cell and that expected theoretically. An absorbent layer of incorrect thickness can disrupt this correspondence. Thus, the form factor is largely affected as the thickness becomes greater and greater. An efficiency of nearly 18.50% (Fig. 3c) is obtained for thicknesses between 0.05 and 0.5 μm and drops off above 0.5 μm . Increasing the thickness of the absorber leads to an increase in the recombination rate in the cell. Thus, an ultra-thin thickness is required to increase the electric field and facilitate the collection of charge carriers.

Influence of the Length of Carrier Diffusion in the Absorber

The carrier diffusion length determines the distance the carriers can travel before recombining and will therefore significantly impact the cell's performance. Assuming that the effective electron capture cross-section and the holes are identical, the diffusion length of the electrons is equal to that of the holes. This relationship is given by:

$$L_n = L_p = \sqrt{\frac{D_{n,p}}{\sigma_{n,p} v_{thn,p} N_t}} \quad (4)$$

where,

- $\sigma_{n,p}$ = The effective electron or hole capture cross-section
- $v_{thn,p}$ = The thermal velocity of the electrons and holes
- $D_{n,p}$ = The diffusion constant, which is related to carrier mobility by the Einstein relation

$$D_{n,p} = \frac{kT}{q} \mu \quad (5)$$

In this section, the diffusion constant, capture cross-sections, and thermal velocities are assumed to be constant. Therefore, the diffusion length depends only on the defects in the absorber. The diffusion length was simulated between 0.05 and 2 μm by varying the defect density from 10^{13} - 10^{16} cm^{-3} . Figures (4a-b) shows the influence of the diffusion length on the current-voltage characteristic and quantum efficiency. It can be seen that the diffusion length affects the open circuit voltage (V_{CO}), the circuit current density (J_{SC}), and the collection of charge carriers.

The parameters extracted from the current-voltage characteristic are shown in Fig. 5. All the electrical parameters are affected by the variation in diffusion length. The open-circuit voltage in Fig. (5b) increases sharply for small diffusion lengths of 0.6 μm . Above this value, the V_{CO} stabilizes at 1.03 V. As for the current density (J_{SC}) increases from a diffusion length of less than 0.2 μm and stabilizes at 22.8 mA/cm^2 . Its form factor is 52% for a diffusion length of less than 100 nm. It saturates at 77% for a diffusion length greater than 100 nm. V_{CO} and J_{SC} reach 1.0 eV and 23 mA/cm^2 , respectively, when the scattering length exceeds a certain value of 100 nm. It also appears that the form factor is much more sensitive to variation in diffusion length (Berhe *et al.*, 2016). This could be because the applied electric field to the absorber diminishes. as the direct polarization increases. As a result, the initially supported enhancement of carrier collection due to the electric field diminishes. Conversely, the electric field in the absorber continues to aid in carrier collection in the short-circuit state, resulting in a relatively minor influence of the diffusion length on J_{sc} .

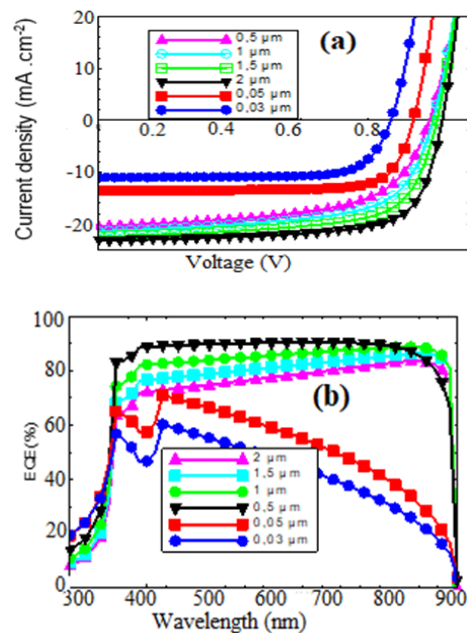


Fig. 2: Influence of absorber thickness on; (a) The current-voltage characteristic and; (b) The quantum efficiency

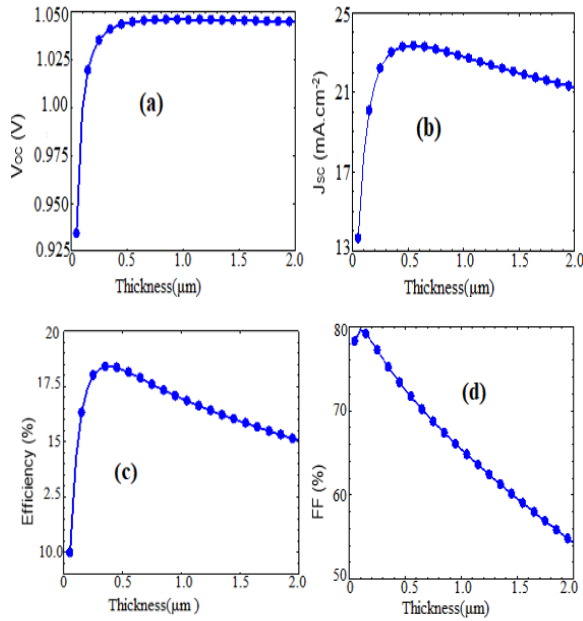


Fig. 3: Influence of absorber thickness on; (a) Open-circuit voltage (V_{oc}); (b) Short-circuit current density (J_{sc}); (c) Conversion efficiency and; (d) Form Factor (FF)

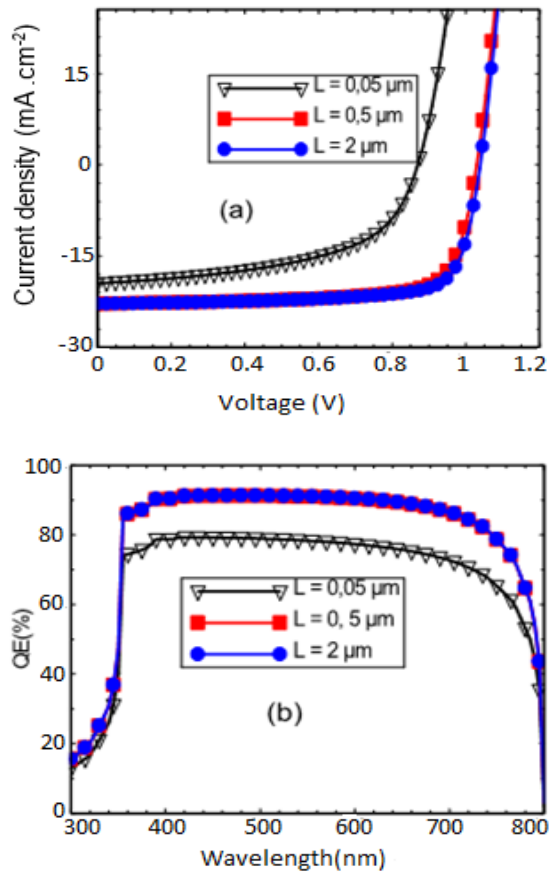


Fig. 4: (a) Current-voltage characteristic; (b) Quantum efficiency as a function of diffusion length

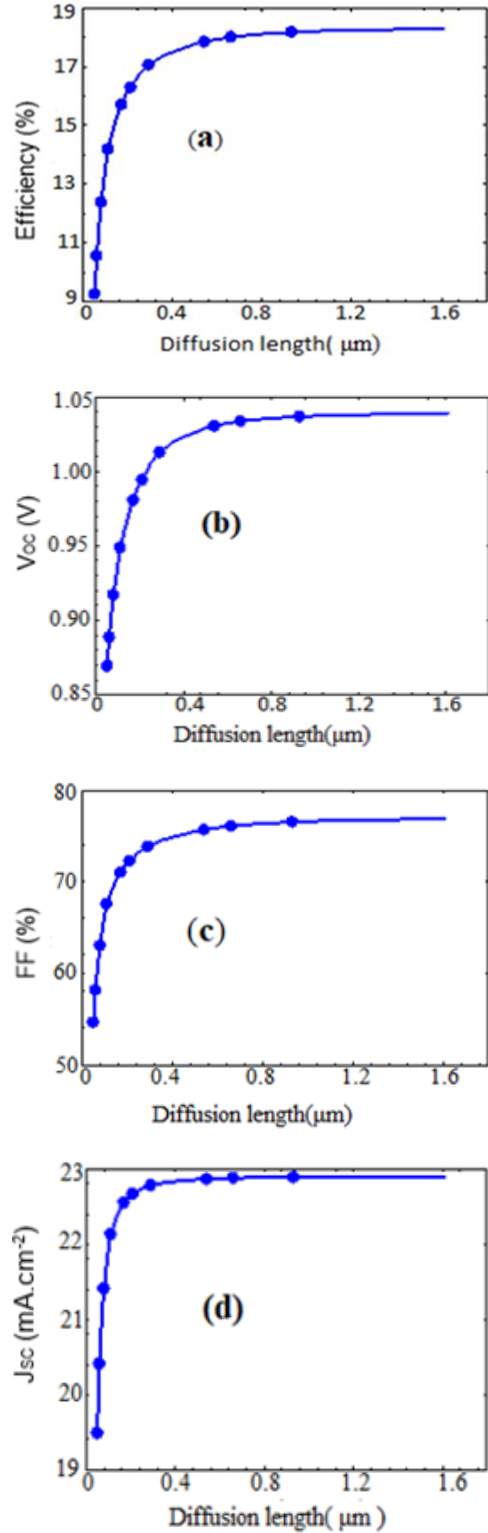


Fig. 5: Curves illustrating the influence of the carrier diffusion length in the absorber as a function of the electrical parameters; (a) Conversion efficiency; (b) Open-circuit voltage (V_{oc}); (c) Form Factor (FF); (d) Short-circuit current density (J_{sc})

Influence of Charge Carrier Lifetime

In this section, we analyze the influence of charge carrier lifetime and thickness on the electrical parameters. For this simulation, we varied the absorber thickness from 0.03-2 μm and the defect density from 10^{14} - 10^{17} cm^{-3} . Figure 6 shows the evolution of the electrical parameters when the two parameters are varied simultaneously. Since the lifetime depends on the diffusion length, the more the absorber thickness is reduced, the smaller the generation current, which has an impact on the short-circuit current density. Unlike J_{sc} , the Form Factor (FF) diminishes as the absorber thickness increases, irrespective of the quality of the absorber. Increasing the absorber's thickness leads to a decrease in the electric field within the absorber and consequently, the Form Factor (FF) when the absorber is of poor quality, i.e., a lifetime of less than $1.6 \cdot 10^{-2} \text{ ns}$. Even in the case of a high-quality

absorber, a reduction in FF occurs as the absorber thickness increases. The trend in V_{oc} is almost similar to that of FF. The slight enhancements in V_{oc} for a lifetime corresponding to $5.1 \cdot 10^{-1} \text{ ns}$ the marginal rises in V_{oc} can be attributed to the heightened J_{sc} , as V_{oc} is determined by the equilibrium between the generation current and the recombination current. These findings suggest that the ideal thickness depends on both light absorption and absorber quality and it is essential for absorber quality to meet a certain level to optimize cell performance (Wu *et al.*, 2016; Xing *et al.*, 2016).

Influence of Defect Densities at Interfaces

Interface quality is an essential parameter for achieving high efficiency in thin-film solar cells (Fakharuddin *et al.*, 2017; Yan *et al.*, 2015). Quantifying the impact of interface defects is very difficult experimentally.

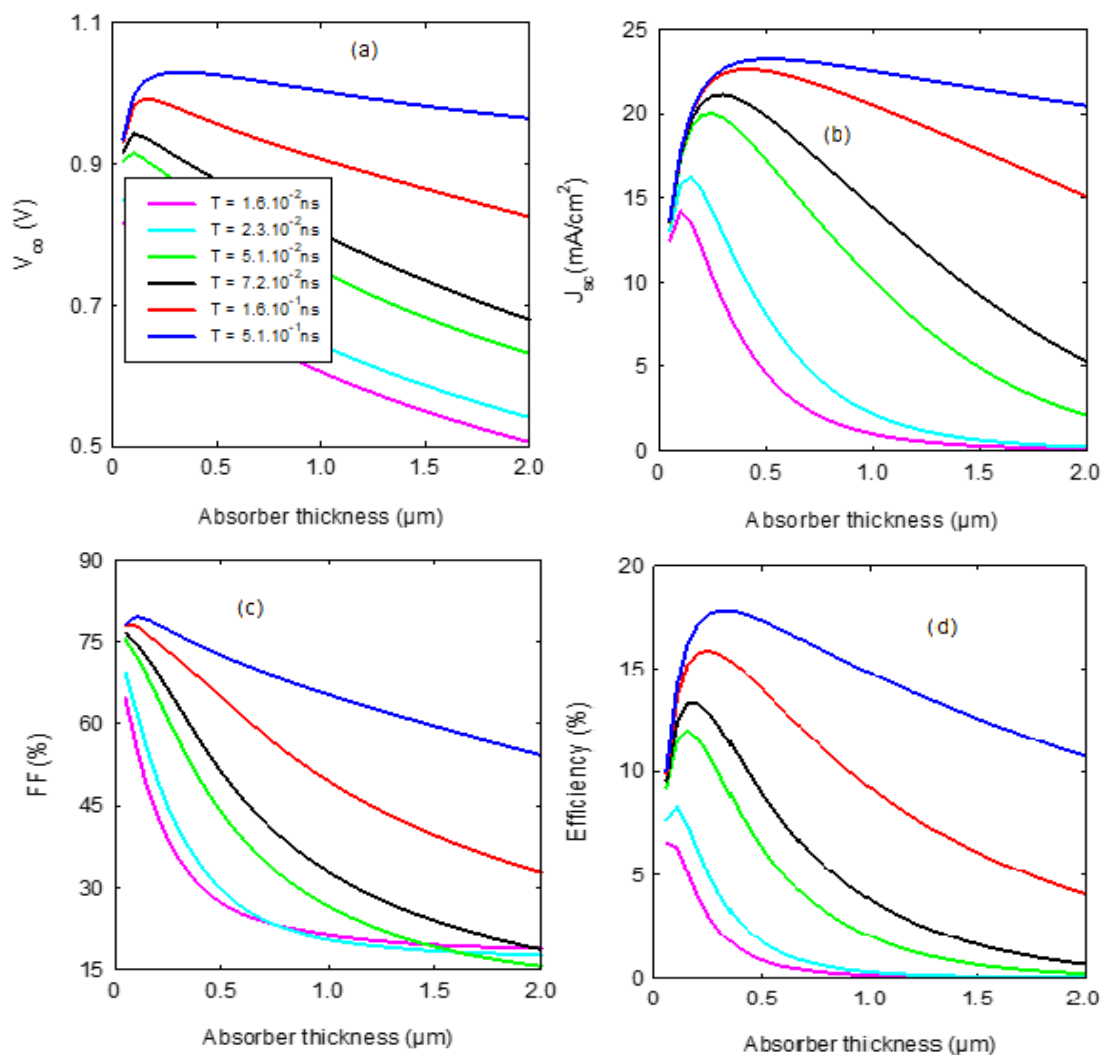


Fig. 6: Influence of charge carrier lifetime and thickness on electrical parameters; (a) V_{oc} ; (b) J_{sc} ; (c) FF; (d) Efficiency

Therefore, we varied the defect density at the TiO₂/perovskite interface (IDL1) and the perovskite/HTM interface (IDL2) from 10¹³-10¹⁸ cm⁻³ to shed light on the impact of interface quality on device performance. On the other hand, Fig. (7a). Suggests that the efficiency is significantly influenced by the defect density at the interface between the buffer layer and perovskite, and enhancing the quality of this interface could lead to an efficiency greater than 21%. Figure 8 shows that the electrical parameters all vary linearly when the interface defect density is between 10¹³ and 10¹⁷cm⁻³. Beyond this range, all the parameters fall as the defects in the IDL1 and IDL2 layers increase.

Figure 7 Current-Voltage (J-V) characteristics of perovskite solar cells with varying defect densities at the; (a) Buffer/absorber interface (IDL1); (b) Absorber/HTM interfaces (IDL2). We also note that the quality of the interface between the buffer layer and the absorber has a more pronounced influence on the parameters compared to the interface between the absorber and the HTM (Fig. 8). For a defect density equal to 10¹⁵ cm⁻³ in the IDL1 and IDL2 layers, the decrease in electrical parameters due to recombination's in the IDL2 layer are $\Delta V_{oc} = 0.01$ V; $\Delta J_{sc} = 0.8$ mA/cm²; $\Delta FF = 4\%$ and $\Delta \eta = 1.6\%$. At first sight, one might think that the difference in fault density influences would be due to the presence of the buffer layer.

However, when the simulations are carried out without the buffer layer, the results are similar. The variation in the influence of interface defect densities can be attributed to recombination processes (Minemoto and Murata, 2014a). When the cell is exposed to light, it generates electron-hole pairs and there is a greater concentration of these pairs at the surface than at the back contact. Thus, as the front of the cell is rich in electron-hole pairs, interface defects in the IDL1 layer will have an enormous impact on the electrical characteristics.

Figure 9 shows that J_{sc} increases with thickness, due to the increase in the absorber layer. On the other hand, it

affects the open-circuit voltage V_{co}, the Form Factor (FF), and the efficiency when it becomes large. One of the causes of this variation could be the high density of defects in the absorbing layer. These defects affect the lifetime of the carriers by preventing them from being collected efficiently.

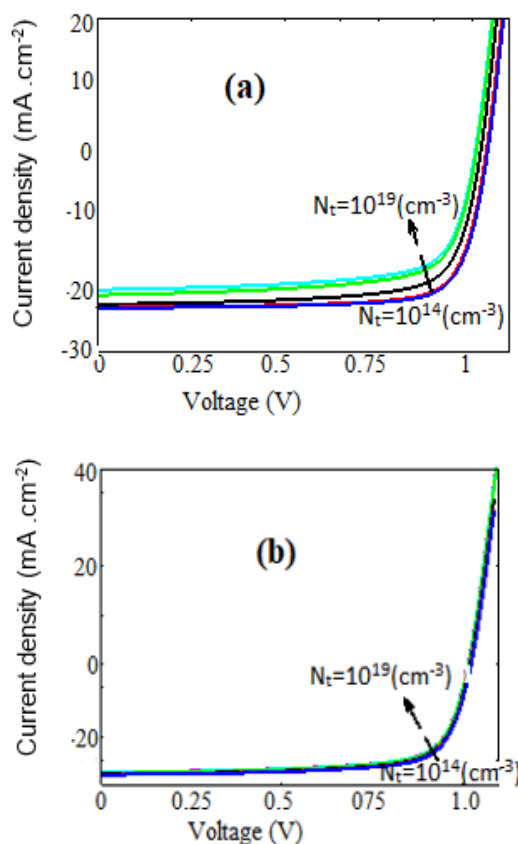
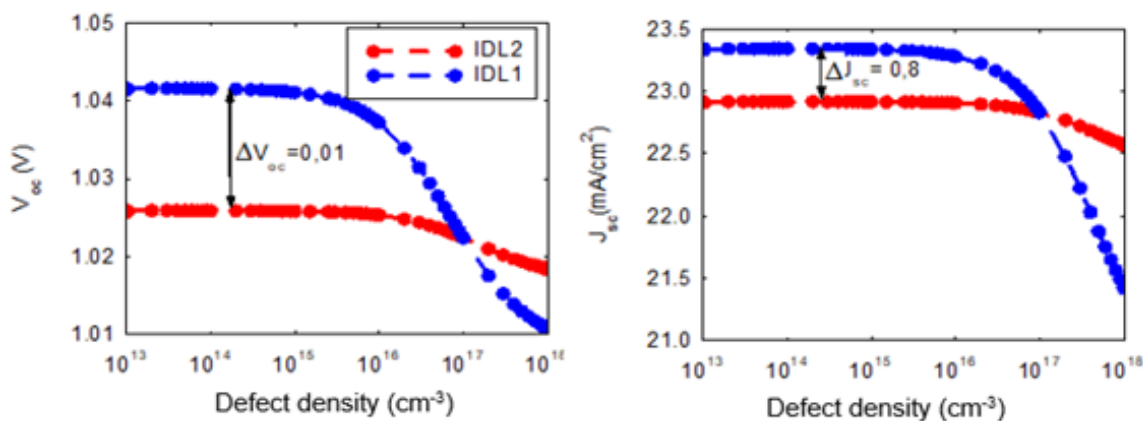


Fig. 7: (a-b) shows the influence of the defect density in the IDL1 and IDL2 layers on the current-voltage characteristic. On the one hand, it can be seen that the two J-V curves are almost identical when the defect density varies from 10¹⁴-10¹⁹cm⁻³



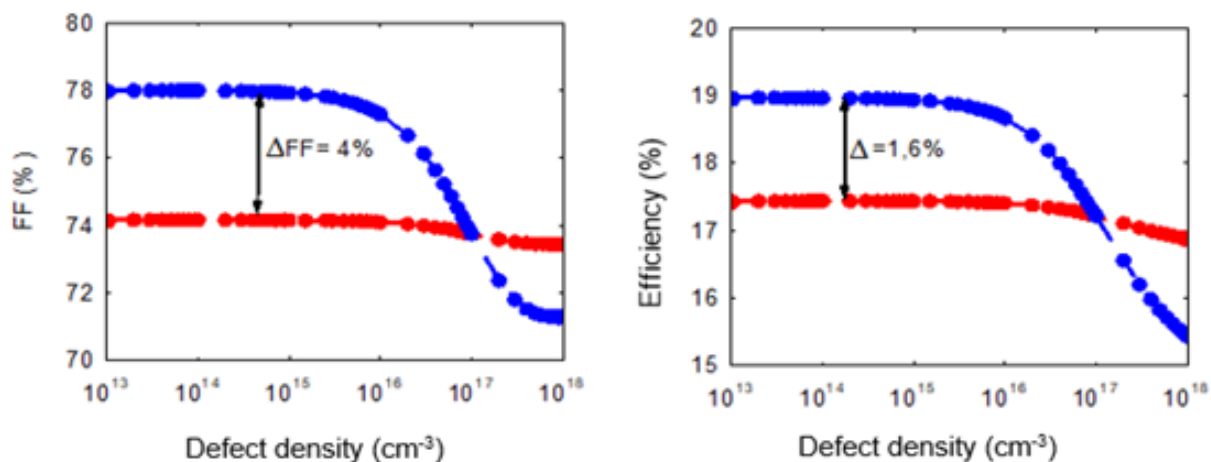


Fig. 8: Influence of defect density at the buffer layer/absorber interface (IDL1) and at the absorber/HTM interface (IDL2) on the electrical parameters

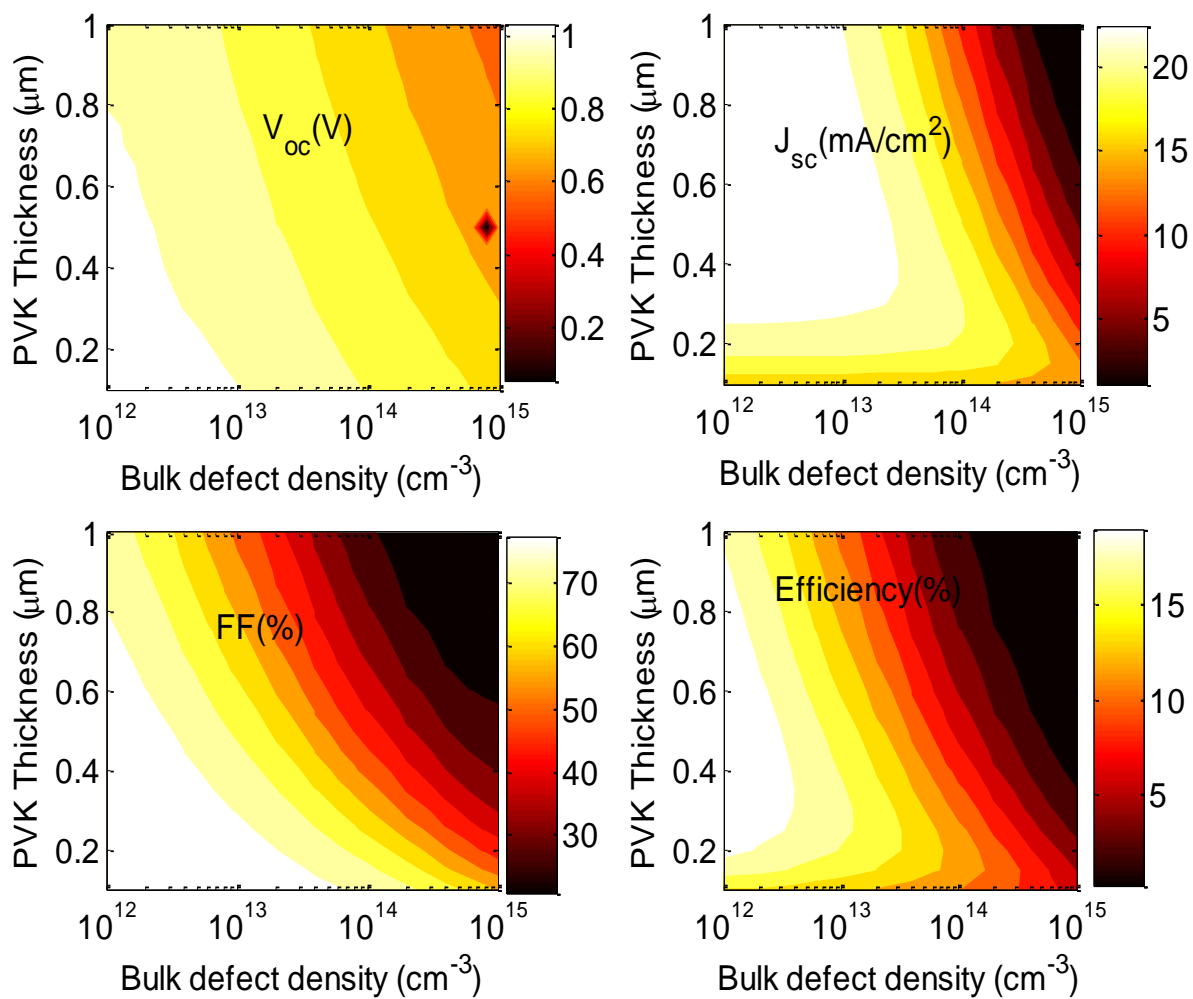


Fig. 9: Curves illustrating the variation in electrical parameters as a function of increasing absorber layer thickness and defect density

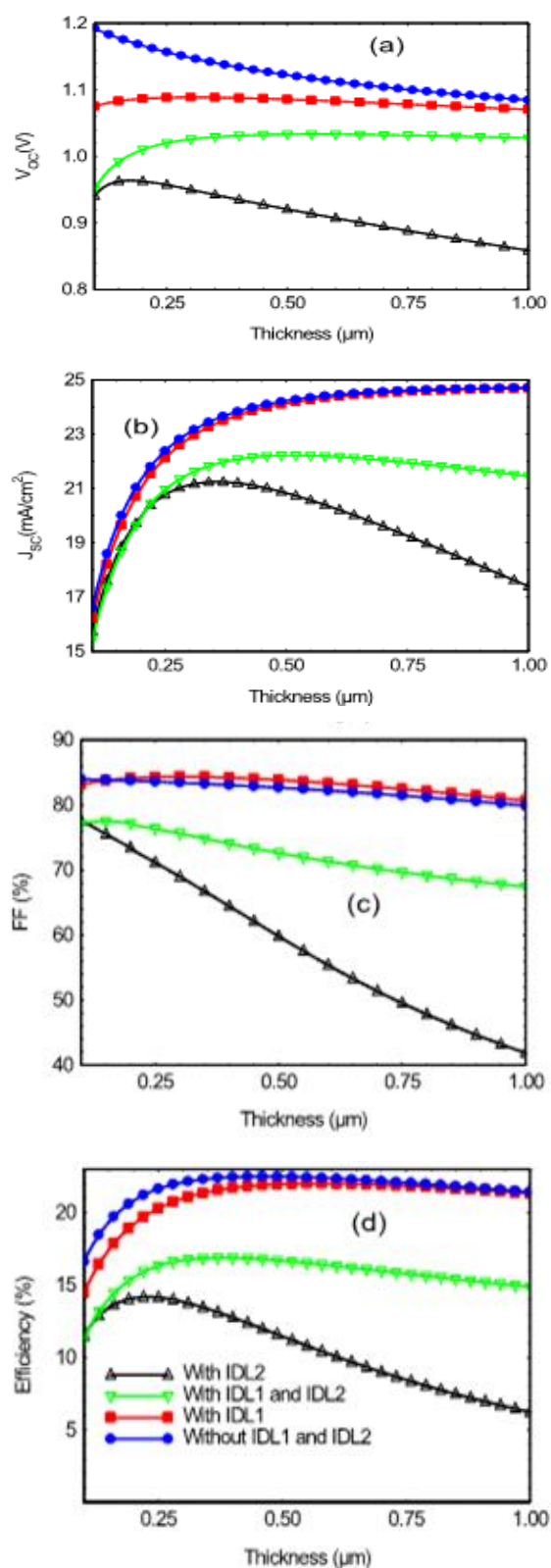


Fig. 10: Curves illustrating the impact of the IDL1 and IDL2 layers on the variation in electrical parameters as a function of thickness

Influence of the IDL1 and IDL2 Layers on the Variation of Electrical Parameters as a Function of Thickness

Figure (10a) shows an open-circuit voltage V_{CO} that reaches a maximum value ($V_{CO} = 1.2$ V) without the IDL1 and IDL2 layers and decreases progressively with thickness and a quasi-linear voltage ($V_{CO} = 1.1$ V) with the IDL1 layer at the buffer/absorber layer interface, while V_{CO} stabilizes at 1.0 V with the IDL1 and IDL2 layers. On the other hand, V_{CO} drops drastically with the IDL2 layer at the absorber/HTM interface. In Fig. 10b we have a current density $J_{SC} = 24$ mA/cm² both with the IDL1 layer between the buffer/absorber interface and without the IDL1 and IDL2 layers, however, with only IDL1 and IDL2 it saturates to 22 mA/cm² and drops sharply with IDL2 between the absorber/HTM interface with the change in thickness. The curves (Fig. 10c-d) show a form factor of 85% and an efficiency of 22% with and without the IDL1 and IDL2 layers. In contrast, the form factor is 78% and the efficiency is 15% with the IDL1 and IDL2 layers only at the interfaces, while the form factor and efficiency drop sharply with the IDL2 layer at the absorber/HTM interface. We note that the IDL1 and IDL2 layers do not have a major influence on the open-circuit voltage of the (V_{CO}), but the current density and form factor require a good quality absorber for good charge carrier collection.

Conclusion

In this study, we have focused our research on perovskite-based solar cells and proposed some ways to improve their efficiency. Our simulation results show that the thickness, lifetime, and diffusion length of charge carriers are interdependent parameters that need to be carefully tuned to optimize the performance of perovskite solar cells. The results suggest that the use of a 0.5 μm active layer can lead to an optimization of the electrical parameters and allow the design of good-quality solar cells. The aim is to achieve a balance between maximum light absorption, high conversion efficiency, and minimization of losses due to charge carrier recombination. Research must continue to better understand these parameters and optimize them to further improve perovskite solar cells.

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Author's Contributions

Issiaka Sankara, Soumaïla Ouédraogo and Daouda Oubda: Conceptualization, methodology, software, written-original drafted preparation.

Boureïma Traoré, Marcel Bawindsom Kébré and Adama Zongo: Data curation, methodology, software and original drafted.

François Zougmore: Written-reviewed and edited, supervision, validation, project administration.

Ethics

The corresponding author declares that this manuscript is original and has not been published before. I can confirm that the manuscript has been read and approved by all named authors.

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