Power, Energy and Electrical Engineering
M. Deng (Ed.)

doi:10.3233/ATDE240354

Performance Optimization of Double-Absorber Perovskite Solar Cell: Numerical Calculations

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Abstract. In this study, we designed and simulated a new double absorber perovskite solar cell device by performing numerical analysis using SCAPS-1D. The architecture of the solar cell device consists of Glass/FTO/C_2N/$CsSnGeI_3$/$CsSnI_3$. Optimizing the core parameters of CsSnGeI3 implied to an encouraging solar cell performance with a remarkable power conversion efficiency of 28.61%. The results show that increasing the thickness of $CsSnGeI_3$ to 1000 nm enhances the solar cell performance. The simulations show that increasing the absorber layer thickness is desirable to promote the spectrum absorption process, thus accelerating the generation rate of the charge carriers. Increasing the doping density in $CsSnGeI_3$ implied to inconsistent impact on the solar cell performance. The solar cell displayed the optimal performance at low and high doping level, while at intermediate doping level, the solar cell efficiency depreciates to 23.18%. This result is ascribed to creation unstable depletion regions at this doping level, which prevent the charge carriers from reaching the metal back contact. Additionally, increasing the defect density in $CsSnGeI_3$ yielded a sharp continuous degradation in the device performance. The power conversion efficiency decreased to 15.22%. Finally, increasing the operating temperature showed a harsh impact on the solar cell performance, and the optimal performance occurs at 300 K. It is believed that the simulated model represents an added value and a great potential in the field of solar cells research and fabrication.

Keywords. double-absorber, perovskite, efficiency, SCAPS

1. Introduction

Nowadays, perovskite materials attract an enormous interest as a solar energy harvester in the solar cells markets. Their excellent optoelectronic properties, simple fabrication processes and low-cost raw materials qualified them as pioneer materials for optoelectronic devices [1-2]. Over the past years, a large number of perovskite materials have been produced, developed and implemented in solar cells devices, resulting in a pronounced progress in achieving high solar cell performance [3-4]. However, most

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studies on perovskites were limited on implementing these materials as a single absorber layer in the solar cell structure, which implied to a limited solar cell performance. Recently, a large number of studies have considered impact of using double absorber layer [5-6]. They have reported a pronounced progress in the solar cell performance upon implementing double absorber layer in the solar cell structure. A recent study has shown an efficiency of 32.42% in $NaZn_{0.7}Cu_{0.3}Br_3/MASnI_3$ double-absorber solar cell [7].

Despite this progress for perovskite materials, many of them are toxic and show instability in their structure, which limits their potential expansion in solar cell devices [8-9]. Therefore, adopting the echo-friendly perovskite material in the solar cell is crucial for the commercialization process. Among several perovskite materials, $CsSnGeI_3$ and $CsSnI_3$ appeared recently as a strong absorber layer candidates for solar cells. They are characterized by a narrow energy band gap (1.5 eV for $CsSnGeI_3$ and 1.3 for $CsSnI_3$) which grantee an absorption process for a broad wavelength range in the visible spectrum. Raghvendra et.al. has reported a solar cell efficiency of 13.29% upon using $CsSnGeI_3$ as a single absorber layer [10]. I. N. Khan et. al. has achieved recently an efficiency record of 27.21% in $CsSnGeI_3$ perovskite solar cell with TiO_2 and CNTS as charge transport layers [11]. On the other side, B. K. Ravidas et. al. has reported a solar cell efficiency of 26.4% in $CsSnI_3$ based perovskite solar cell [12].

In this study, we report optoelectronic simulation results on a new solar cell structure based on $CsSnGeI_3/CsSnI_3$ as a double-absorber layer in the solar cell structure using one dimensional solar cell simulation software (SCAPS) [13]. The current study is limited on optimizing the $CsSnGeI_3$ core parameters such as the thickness, doping density and defect density. In addition, the effect of the operating temperature of the device is studied. We believe strongly that the output of this study will have a strong impact on solar cells research.

2. Research Methodology

Numerical analysis is a crucial step in solar cell research. It gives a comprehensive picture of the device's performance before proceeding with fabrication. Among several available software for solar cell simulation, the solar cell capacitance simulator software (SCAPS) has proven its capability as an experienced software for solar cell investigations [13-17]. SCAPS-1D is performed by considering three different differential equations namely Poisson's equation, continuity equation for electrons, and holes. Poisson's equation is given in (1).

$$\frac{\partial^2\psi}{\partial^2\psi} + \frac{q}{\epsilon}\left[p(x) - n(x) + N_D - N_A + p_p - p_n\right] = 0 \quad (1)$$

Perovskite solar cells (PSCs) rely on both electron and hole charge carriers, and their output current is determined by the contribution of both diffusion and drift mechanisms. The hole continuity equation is given in (2).

$$\frac{1}{q}\frac{\partial J_p}{\partial x} = G_{op} - R(x) \quad (2)$$

The electron continuity equation is given in (3).

$$\frac{1}{q}\frac{\partial J_n}{\partial x} = -G_{op} + R(x) \quad (3)$$

where Ψ represents the electrostatic potential, N_A and N_D are the acceptor and donor density respectively. ρ_p and ρ_n are used as the hole and electron distribution, respectively. J_p and J_n are the current density due to holes and electrons, respectively. G_{op} is the carrier generation rate, and R is the total recombination rate [13].

In this study, numerical calculations were done using SCAPS to explore the optoelectronic performance of $CsSnGeI_3$/$CsSnI_3$ double-absorber perovskite-based solar cells. Fig.1 shows the device structure and the corresponding energy band diagram. The solar cell is based on $CsSnGeI_3$ and $CsSnI_3$ perovskite materials as absorber layers. Fluorine-doped tin oxide (FTO) and Carbon Nitrate (C_2N) are implemented in the device structure as window and buffer layers, respectively. Silver is considered a metal back contact layer. In SCAPS, the material properties of each layer must be manually inputted. Therefore, selecting these parameters is crucial for achieving accurate simulation results. Table 1 lists all initial input parameters used in the simulation for all layers. All parameters are taken from several previous novel studies [17-20]. The photovoltaic properties of open-circuit voltage (Voc), short-circuit current density (Jsc), Fill Factor (FF), and power conversion (PCE) have been investigated at 300 K and under AM 1.5 spectrum and one sun. The initial simulation results have shown a promising solar cell performance. As shown in Fig. 2, the Jsc hits 21.62 mA/cm^2, and the quantum efficiency (QE) displays an active behavior within the visible wavelength range of 300 nm to 900 nm. The QE approaches around 99% at 340 nm. The initial simulation resulted in a PCE of 21.31%, Voc of 1.12 V, and FF of 88.66%. These results strongly indicate realistic input parameters for the solar cell device and agree well with the reported results on $CsSnGeI_3$ based solar cells [10-12]. In this study, we confined our investigation to varying the thickness, doping, and defect density of the $CsSnGeI_3$ layer and the operating temperature to identify the optimal input parameters for the device's performance.

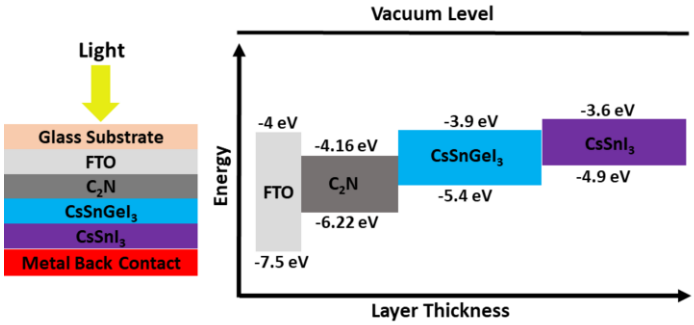

Figure 1. Solar cell configurations and the corresponding energy band diagram.

Table 1. List of input parameters

Parameters	FTO	C_2N	$CsSnGeI_3$	$CsSnI_3$
Thickness (nm)	100	300	0.5	500

Band gap (eV)	3.5	1.8	1.5	1.3
Electron affinity (eV)	4.0	4.2	3.9	3.6
Dielectric Permittivity	9	4.5	28	9.9
CB effective density of states (cm^{-3})	2.2×10^{18}	1×10^{19}	3.1×10^{18}	1×10^{19}
VB effective density of states (cm^{-3})	2.2×10^{18}	1×10^{19}	3.1×10^{18}	1×10^{18}
Electron thermal velocity (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Hole thermal velocity (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Electron mobility (cm^2.V.s)	20	13	974	1.5×10^{3}
Hole mobility (cm^2.V.s)	20	20.6	213	5.8×10^{2}
Donor doping concentration (cm^{-3})	2×10^{19}	1×10^{15}	0	0
Acceptor doping concentration (cm^{-3})	0	0	1.1×10^{19}	1×10^{20}
Defect density N_t (cm^{-3})	1×10^{14}	1×10^{14}	1×10^{14}	1×10^{14}

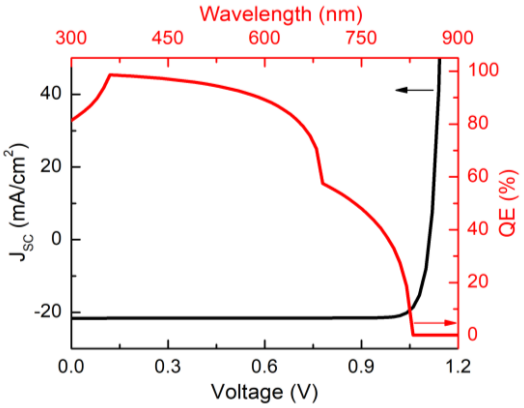

Figure 2. Initial short circuit current density – voltage (J_{sc}-V) and Quantum efficiency (QE) characteristics.

3. Results and Discussion

3.1. Impact of the Absorber Thickness

The thickness of the absorber layer is one of the significant parameters that resolve the solar cell's performance. The layer is a factory for the photogenerated charge carriers

inside the solar cell. Several studies have reported that the optimal performance for the solar cell occurs at a critical thickness [21-23]. The correlation between the solar cell performance and the absorber layer thickness can be explained through its impact on the diffusion length of the photogenerated charge carriers. As the absorber layer thickness increases, many photons responsible for generating the charge carriers with higher diffusion lengths will be absorbed. However, large thickness values could result in the solar cell performance degradation due to an increase in the reverse saturated photocurrent. To find out the best performance for our designed solar cell device, the thickness of $CsSnGeI_3$ has varied from 100 nm to 1000 nm, keeping all other parameters fixed at their initial values. Fig. 3 (a-d) shows the impact of the thickness change on the optoelectronic performance parameters. All parameters increase with increasing the absorber layer thickness. The fill factor displayed a slight positive change with increasing thickness. This positive change in all parameters indicates increased photogenerated charge carriers inside $CsSnGeI_3$. At 1000 nm, the solar cell displayed optimal performance with PC, keeping all other parameters fixed at their initial values. Fig. 3 (a-d) shows the impact of the thickness change on the optoelectronic performance parameters. All parameters increase with increasing the absorber layer thickness. The fill factor displayed a slight positive change with increasing thickness. This positive change in all parameters indicates increased photogenerated charge carriers inside $CsSnGeI_3$. At 1000 nm, the solar cell displayed the optimal performance with PCE of 24.45%, Voc of 1.13 V, Jsc of 24.28 mA/cm^2, and FF of 88.66%.

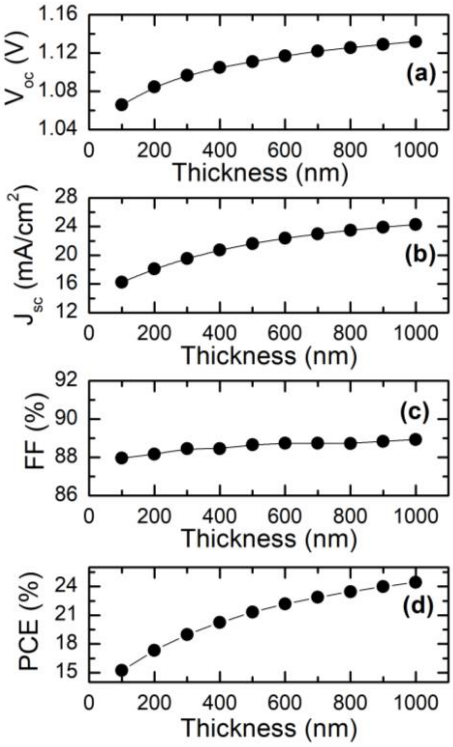

Figure 3. Impact of the $CsSnGeI_3$ thickness on the optoelectronic performance parameters.

3.2. Impact of the Absorber Doping Density

The impact of the absorber layer doping density on the solar cell performance is very crucial. Increasing the doping density to a certain level could enhance or decrease the solar cell performance [24-25]. In this stage of our study, optimization of the device through the doping density was done for $CsSnGeI_3$. The doping rate has been varied from 1×10^{13} cm^{-3} to 1×10^{22} cm^{-3} at the optimal thickness of 1000 nm and all other parameters were kept fixed at their default values. As displayed in Fig. 4, the power conversion efficiency (PCE) stayed almost at a stable level of 27.89% in the doping range 1×10^{13} cm^{-3} to 1×10^{15} cm^{-3}. Beyond 1×10^{15} cm^{-3}, a sharp drop in solar cell efficiency down to 23.18% at doping level 1×10^{15} cm^{-3}, followed by an increase in the PCE to a value of 28.61% at doping density of 1×10^{22} cm^{-3}. This observation could be due to the building of unstable depletion regions at this doping level leading to the production of a built-in voltage, which works as a trapping area for the charge carriers to reach the back contact. However, it gets clearer that low or high doping levels are more favorable for promoting solar cell performance.

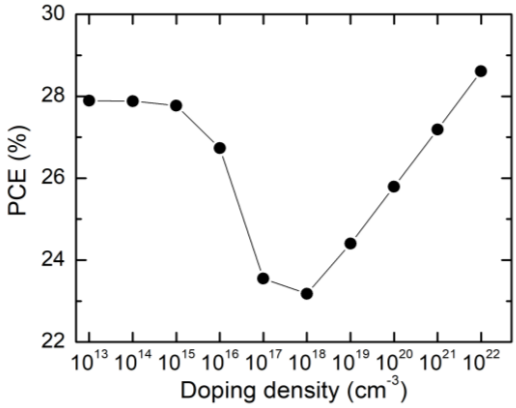

Figure 4. Impact of the $CsSnGeI_3$ doping density on the power conversion efficiency (PCE).

3.3. Impact of the Absorber Defect Density

In perovskite solar cells, like other layered solar cells, the quality of layers is essential for promoting the performance of the solar cell device. The defects play as trapping centers and accordingly accelerate the recombination rate of the photogenerated charge carriers. This feature is known to prevent the carriers from reaching the metal back contact. As a result, this causes a depreciation in the device's performance. As reported, the defects can be found in perovskite materials in several forms, such as point defects, Frenkel defects, and dislocations and boundaries [26-27]. In this study, the effect of the defect density of $CsSnGeI_3$ on the optoelectronic parameters is investigated. For this purpose, the defect density was varied from 1×10^{13} cm^{-3} to 1×10^{21} cm^{-3}. The obtained results are illustrated in Fig. 5. As shown in Fig. 5, the solar device displayed the highest performance at a defect density of 1×10^{13} cm^{-3} with PCE of 28.61%, J_{sc} of 24.24 mA/cm^2, V_{oc} of 1.1.31 V, and FF of 90.18%. As the defect density increases, all parameters drop sharply. The PCE drops to 15.22% at a defect density of 1×10^{21} cm^{-3}. This deterioration

in the solar cell performance is attributed to the reduction in the photogenerated charge carriers' lifetime and diffusion length, which prevent them from reaching the metal back contact.

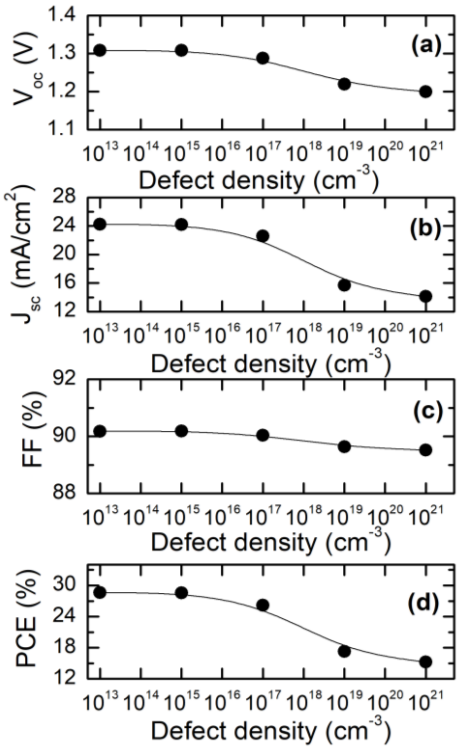

Figure 5. Impact of the $CsSnGeI_3$ defect density on the optoelectronic performance parameters.

3.4. Impact of Operating Temperature

Solar cell structure is highly affected by temperature change. Increasing the temperature could cause a deformation between layers. This deformation creates interfacial defects between the layers, which work as trapping centers that reduce the diffusion length of the charge carriers, and this prevents them from reaching the metal back contact. As a result, a depreciation in the solar cell performance. Several studies have reported this negative impact of the temperature on solar cell performance [28-29]. To examine this effect on our modeled device, the temperature was varied from 300 K to 500 K. As shown in Fig. 6, the solar cell shows poor performance with the temperature increase. The PCE dropped from 28.61% to 20.29%. This poor performance could be attributed to poor interconnectivity between layers.

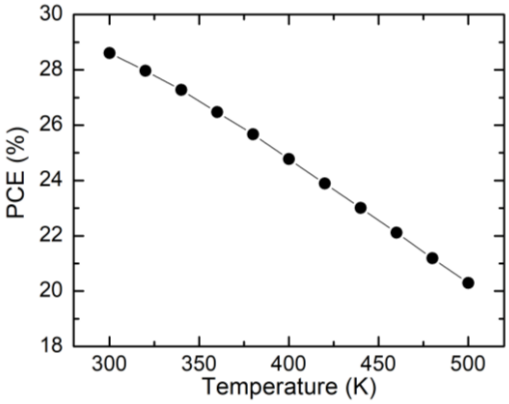

Figure 6. Impact of the operating temperature on the solar cell performance.

3.5. Conclusions

In this research, we modelled and simulated a new double absorber solar cell device based on perovskite materials. All simulations were performed by utilizing the SCAPS-1D. The current study confined on optimizing the core parameters such as the thickness, doping density, and defect density of the absorber layer $CsSnGeI_3$ as the first stage. Careful optimization of the core parameters of $CsSnGeI_3$ implied to a promising solar cell performance with an efficiency record of 28.61%. The results showed that optimizing the thickness for $CsSnGeI_3$ was crucial for enhancing the solar cell performance. The optimized thickness for $CsSnGeI_3$ was at 1000 nm. The doping density in $CsSnGeI_3$ showed a significant irregular impact on the device performance. The solar cell displayed high performance at low and high doping levels. At intermediate doping levels (1×10^{15} - 1×10^{18} cm^{-3}), a degradation in the performance is observed. These finding is argued to creation unstable depletion regions at this intermediate doping level, which obstacle the photogenerated charge carriers from reaching the metal back contact. The defect density in $CsSnGeI^3$ impacted the device performance negatively. Increasing the defect density resulted in depreciation the device performance. Finally, the operating temperature appeared a harmful effect on the solar cell performance, and the device works optimally at 300 K. We believe that investigating the optoelectronics parameters for other layers in the structure could lead to a higher performance for the solar cell through parameters optimizations. In addition, the current modelled solar cell concludes a great potential toward the fabrication of high-efficiency perovskites-based solar cell devices.

Acknowledgment

The authors are thankful to Marc Burgelman, the Electronics and Information Systems (ELIS), University of Gent, Belgium, for providing free access to SCAPS-1D simulation software.

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