Nano World Journal

https://doi.org/10.17756/nwj.2023-s5-021

Research Article

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Comparing the Performance of Lead-based and Lead-free Inorganic Perovskite Solar Cell Using SCAPS-1D

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Received: October 11, 2023
Accepted: December 19, 2023
Published: December 22, 2023

Citation: Jeepa KJ, Subash TD, Samy JWK. 2023. Comparing the Performance of Lead-based and Lead-free Inorganic Perovskite Solar Cell Using SCAPS-1D. *NanoWorld J* 9(S5): S106-S108.

Published by United Scientific Group

Abstract

In perovskite solar cell (PSC) research fields organic-inorganic lead halide planar architectures are becoming popular as they are useful and workable for tandem structure easier fabrication process and low temperature processability. The commonly examined charge transport materials are organic for planar or inverted planar cells, as it affects from poor conductivity, poor chemical stability, and higher processing cost. In order to get better of the limitation of organic equivalent leads towards advancing regards in applying solution processed inorganic metal oxide transport layers up to definite level. Here in lead-based PSC structure and lead-free based PSC, studied about the achievement of electron transport materials ZnO (zinc oxide) and NiO_x (Nickel oxides) as hole transport material (HTM). The open circuit voltage (V_{OC}), short circuit current (J_{SC}), fill factor (FF) and power conversion efficiency (PCE) are thoroughly analysed. The aim of this paper is to presents a comparison between methyl ammonium lead iodide ($CH_3NH_3PbI_3$) based PSC structure and inorganic Cs_2TiBr_6 based PSC structure with NiO_x is used as a hole transport layer and ZnO is used as an electron transport layer. To study the performance of both the PSC structure, a simple but comprehensive ID simulation is used.

Keywords

Perovskite solar cell, Hole transport layer, Electron transport layer, Power conversion efficiency

Introduction

In the future photovoltaic technology has become a promising technology by depletion of fossil fuels [1]. Nowadays more advancements are being reported in solar cell technology, the requirement of most economical, efficient, green, and ample obtainable materials remains a challenge [2]. Compared to ordinary energy sources the best extensively available photovoltaic material is silicon solar cells, but it is not economical [3]. The performance of PSC materials is more and also economical. PSCs are processed at room temperature the PCE of PSCs is increasing from a few to more than 25% in a very small-time span [4]. Among the perovskite materials lead based metal halide perovskite have higher PCE and they become more attractive. Moreover, planar configurations of perovskites are smoothing the way for tandem junction cells [5]. There are two planar architectures n-i-p and p-i-n. But the inverted configuration remains admirable due to the processing feasibility at and T < 150 °C [6], lower hysteresis [7] and better carrier collection capability [4]. The p-type oxide has high bandgap and for incoming light NiO_x contributes better optical transparency, it is selected as HTM and ETM is selected as ZnO, an oxide with higher conductivity [8].

The performance of solar cell parameters is comparatively analyzed, consequently supporting an easier however inverted planar PSCs with an all-metal oxide transport layer domain are analysed extensively. The major concern for commercial application is lead-free perovskite absorber but the lead-based perovskite absorber raises injury to human health and the environment [9]. For high-efficiency solar cells the experts are taking a prominent agreement of curiosity in offering and looking over lead-free perovskites [10].

For solar energy application the lead-free PSCs (Cs_2TiBr_6), has remarkable preference as it has an amalgamation of many serviceable property [11]. The environment friendly titanium-based double perovskites have inventive optoelectronic applications [12]. In future Cs_2TiBr_6, has the potential to supplant $CH_3NH_3PbI_3$ perovskite, also it has outstanding optical, electrical, and photovoltaic properties [13, 14]. Due to the presence of titanium in Cs_2TiBr_6 it becomes an admissible and stable perovskite semiconductor [14].

Nanostructured solar cells hold out a lot of hope for novel methods of generating power from solar radiation. These materials tackle some of the major issues that need to be resolved in order to increase solar cells' overall efficiency [15]. They have outstanding surface-to-volume ratios and surface energy for effective changes in the optical and electrical properties of PSCs and efficient sunlight absorption [15]. Graphene and carbon nanostructures like nanotubes (CNTs) have good stability, are inexpensive, and are simple to produce [16]. They have been mentioned as potential substitutes for HTM and counter electrode materials in several solar cell types. One-dimensional carbon materials known as CNTs have recently received a lot of attention due to their excellent electrical, optical, chemical, and mechanical capabilities [16]. Additionally, CNTs have remarkable flexibility and durability, low reflectance, and ease of preparation, among other outstanding qualities. Perovskites with nanoscale internal ordering, perovskite quantum dots, nanoparticles, nanosheets, and nanorods are examples of nanostructured perovskites. By scaling down the bulk perovskite structure to the nanoscale in at least one structural dimension, these materials often referred to as low-dimensional perovskites can typically be imagined [17].

Experimentation

Device structure and simulation methodology

The structure of proposed planar PSC Ag/ ZnO/ $CH_3NH_3PbI_3/NiO_x$/FTO is shown in figure 1a and lead-free based PSC Ag/ ZnO/Cs_2TiBr_6/NiO_x/FTO is shown in figure 1b. This work has been performed using SCAPS-1D tool under AM 1.5G illumination. Ag and FTO are back contacts and metal front contacts, respectively, in the suggested solar cell. The $CH_3NH_3PbI_3$ a lead-based perovskite layer and Cs_2TiBr_6 non-toxic PSC is the fundamental part of photovoltaic devices and also which acts as an absorber layer. The absorber layer seizes photons and transforms it into electron-hole pairs. A sufficient photovoltaic response may be obtained by sandwiching two electrodes and an absorber layer, but in order to attain the finest solar cell performance electrons and holes are expanded uniformly inside the photovoltaic system.

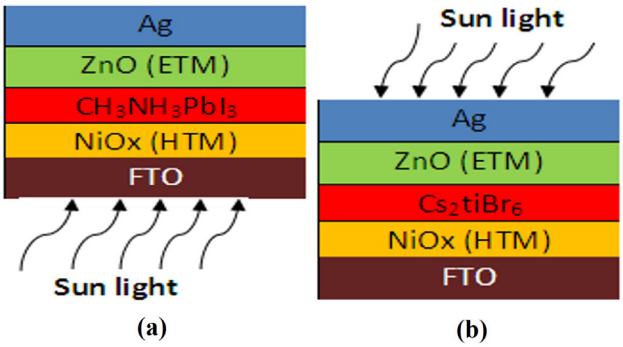

Figure 1: (a) Lead-based PSC and **(b)** Lead-free inorganic PSC.

Results and Discussion

The J_{SC} and V_{OC} characteristics of the proposed two structure is shown in figure 2a and 2b. Table 1 shows the comparison of different parameters of two different PSCs that is one with lead-based and the second one with lead-free, it is noticed that lead-free perovskite material has little higher efficiency than the lead-based PSC.

The highest efficiency is obtained for the absorber thickness of 700 nm. For this thickness the V_{OC} obtained is 1.7813, short circuit current obtained is 23.5 for the FF and PCE of 92.4% and 22.7%, respectively. As the lead-based absorber material is toxic and polluting the environment. So, we can choose the better absorber material which is lead-free and non-toxic.

The thickness of the perovskite layer affects the performance of solar cell and so it is optimized. Figure 3 shows the optimization of thickness of lead-free absorber material. In order to get the optimized thickness, the thickness of the perovskite layer is varied from 700 nm to 1900 nm in simulation and thickness of lead-free absorber material is optimized as 700 nm because best efficiency is obtained for the corresponding thickness and for all other thickness the efficiency is reducing. The output other parameters like V_{OC}, J_{SC}, and FF are also found out in simulation by varying the absorber thickness. For 700 nm, which is the optimized thickness the V_{OC} obtained is 1.20321 V, J_{SC} obtained is 23.302875 mA/cm^2 and the FF is 80.95%. For all other thickness the J_{SC} is increasing, V_{OC} and FF is reducing but here the PCE is considered as great concern and therefore 700 nm is optimized as absorber thickness.

The quantum efficiency of a solar cell is defined as the ratio of the number of electrons in the external circuit produced by an incident photon of a given wavelength. Perovskite absorbing layer can only absorb photons in the range of 790 nm can be more effective (Figure 4).

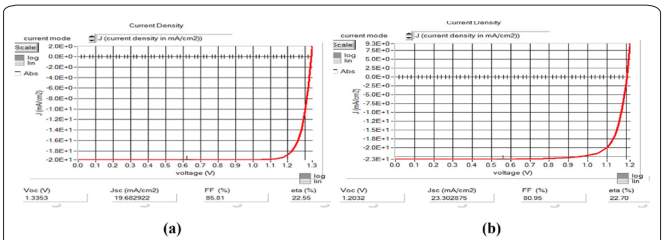

Figure 2: (a) J_{SC} vs V_{OC} characteristics of lead-based PSC and **(b)** J_{SC} vs V_{OC} characteristics of lead-free inorganic PSC.

Table 1: Performance comparison of lead-based and lead-free inorganic PSC.

Perovskite material	V_{OC} (V)	J_{SC} (mA/cm²)	FF (%)	PCE (%)
$CH_3NH_3PbI_3$ (lead-based)	1.335	19.68	85.81	22.55
Cs_2TiBr_6 (lead-free)	1.7813	23.5	92.41	22.7

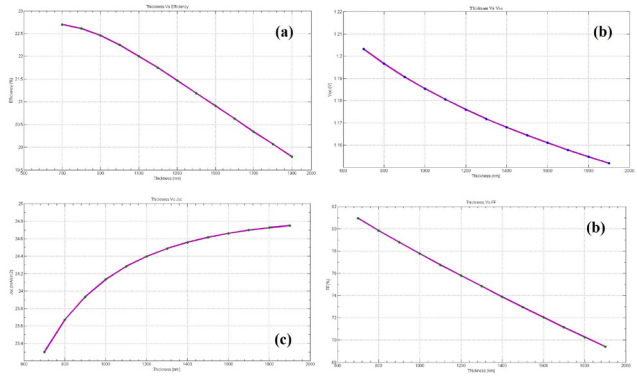

Figure 3: (a) Change in PCE with variation in the thickness of perovskite layer, **(b)** Change in V_{OC} with variation in the thickness of perovskite layer, **(c)** Change in current density with variation in the thickness of perovskite layer, and **(d)** Change in FF with variation in the thickness of perovskite layer.

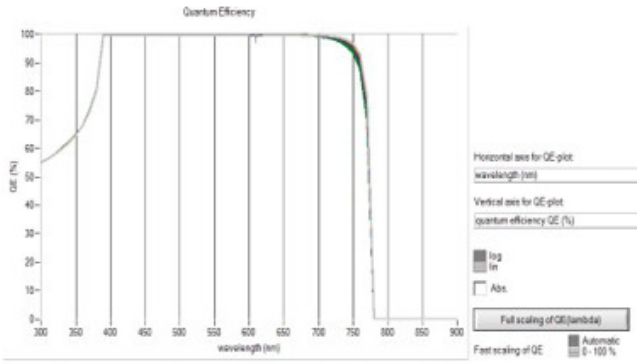

Figure 4: Quantum efficiency of optimized PSC.

Conclusion

In this work, a comparative study of lead-based $CH_3NH_3PbI_3$ and Cs_2TiBr_6 PSC is performed in terms of the photovoltaic parameters. The efficiency attained with lead-based PSC is 22.55% and with lead-free is 22.7%. The inverted planar PSCs imparts an acceptable understanding to these usual inorganic oxides as efficacious carrier transport layers in the simulation-based study. From the simulation study it is analysed that the efficiency of Cs_2TiBr_6 based PSC is little more than the lead-based PSC. The Cs_2TiBr_6 based PSCs are naturally favourable as it is lead-free, so the up-coming technologies may be exploited if we design the structure.

Acknowledgements

None.

Conflict of Interest

None.

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