Theoretical Analysis of Tandem Solar Cell Doped with $MASnI_3$ with P3HT: PCBM Active Layer

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Abstract The organic materials poly(3-hexylthiophene) (P3HT) and (6,6)-phenyl-C61-butyric acid methyl ester (PCBM) are used as the active layer in the tandem photovoltaic structure. Organic solar cells (OSCs) are thin, affordable to create, and hold significant promise for future OSC technological advancement. A tandem cell model consisting of Glass/ITO/PEDOT: PSS/MASnl3/P3HT: PCBM/Al is employed in this study. The P3HT: PCBM is tuned to 220 nm in AM 1.5D and SUN conditions. The efficiency (PCE) was 27.8% and the fill factor was 75%. Scaps-1D is used to model the PCB structure.

Keywords Modeling and simulation · Langevin recombination · Scaps-1D · Solar cell · P3HT: PCBM

1 Introduction

1.1 Perovskite Solar Cells

A kind of solar cell known as a PSC has a perovskite light-absorbing layer. These cells have shown a lot of promise recently due to their great efficiency and inexpensive production costs. These cells' performance and stability can be raised by using methylammonium tin iodide ($MASnI_3$) as the perovskite component. This particular perovskite material's application enables a larger absorption coefficient and increased carrier mobility, which raises the efficiency of power conversion. To increase the long-term stability of these cells, additional study is necessary. A conductive polymer called poly (3,4-ethylene dioxythio-phene): polystyrene sulfonate (PEDOT: PSS)

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R. N. Shaw et al. (eds.), *Innovations in Electrical and Electronic Engineering*, Lecture Notes in Electrical Engineering 1109, https://doi.org/10.1007/978-981-99-8289-9_22

can be used in solar cells to enhance their efficiency. PEDOT: PSS is a semiconductor of the p-type compound which can serve in the role of the hole-transporting film in a solar cell, aiding in raising the collecting and consequently transportation of holes (positively charged carriers) produced by light absorption and boosting the cell's overall efficiency. Perovskite solar cells constructed of methylammonium, lead, and iodine ($MASnI_3$) are one form of solar cell that employs this substance as the active layer to collect sunlight and turn it into energy. These cells are a prospective replacement for conventional silicon-based solar cells due to their high efficiency and low-cost potential. To solve stability difficulties and enhance the effectiveness and stability of these cells, more study is necessary [1, 2]. The production of electricity is essential for the development of the world and is unquestionably the main driver of economic progress in developing as well as developed nations. Massive increases in energy demand are being caused by both increased per capita energy use and rapid population expansion. Fossil fuel-based sources of energy presently provide the majority of the globe's energy needs. Fossil fuel supplies are, however, running out faster as energy use rises. Alternatives to renewable energy must be created in order to address these issues and the growing need for energy. Renewable energy from the sun, which is made up of solar photovoltaic panels that can produce power instantly, is the most abundant renewable energy source. As a substance for photovoltaic light harvesting, perovskite has gained popularity. Thus, lead-based replacements for the metal cations within the perovskite photo-absorber became the main subject of investigation. Group IV of the Periodic Table offers a simple way to substitute lead by stepping up or down. Below the lead in the row is the recently found element, flerovium, which is rarely radioactively stable. Due to its radioactivity, it could not be a practical replacement for lead. Due to its decreased toxicity, tin (Sn), placed on a similar row as lead, may be a suitable alternative for lead in PSCs. Since known of organic tin halide synthesis, natural lead halide synthesis existed [3].

1.2 Literature Review

Having a deficit in energy (Eg) of 1.3 eV, the $MASnI_3$ perovskite was previously claimed to be used in the manufacture of solar cells [4]. Overall, the +2-oxidation property of Sn, thus is necessary to form a perovskite, is fragile; whenever it is subjected to air or oxygen moisture, the element rapidly deteriorates to the +4 state, which affects both the device's working conditions and the method used to create solar cells. Since any contact with oxygen can immediately cause tin oxidation, crystalline tin halide PSCs have been merely tested for functionality alongside rigorous equipment covering [5]. CeO_x is regarded to be among the world's most significant rarest oxides due to its wide bandgap, excellent dielectric properties, and excellent conductivity to ions. By employing a straightforward sol–gel procedure, Wang et al. produced CeO_x ($x = 1.87$) coatings at a relatively low temperature (150 °C) and used them as an alternative to TiO_2 ETL that had undergone a high-temperature annealing process. A champion PCE of 14.32% was achieved by the optimized PSC by altering the CeO_x precursor solution. Yang et al. used $CsPbIBr_2$ perovskite to serve as the light-collecting materials and CeO_x as the electron transfer layer in an inverted PSC arrangement. The all-inorganic PSC reached an all-time high efficiency of 5.6% with improved stability. According to Jien et al., a CeO_x coating acts to provide a perovskite layer of protection that shields the electrode from moisture and metal reactions [6]. The device employing CeO_x to serve as the ETL provides a PCE of 17.47% [7]. Computerized modeling of the photovoltaic cell would prove necessary to establish the right parameters and physical traits for precision in forecasting. The system is emulated by employing the SCAPS-1 D software, and the effectiveness of a tin-PSC is evaluated in relation to changing MASnI3 substrate and CeO_x layer characteristics. FTO/ CeOx/ MASnI3/2,2′,7,7′-tetrakis [N,N-di (4-ethoxyphenyl) amino] is a new device structure. It was previously proposed to simulate a tin-based PSC using the Spiro-OMeTAD using an HTL and 9,9′-spirobifluorene (Spiro-MeTAD)/ Au. This computer model aims to demonstrate how altering the ND values associated with CeO_x and the absorber layer thickness ($MASnI_3$) may enhance the performance of free lead PSCs [8]. In a photovoltaic device, PCBM-doped PEDOT: PSS can function as a reliable transporter for the electron layer. The sunlight-absorbing cell's total efficiency rises as a result of the PCBM molecules' ability to efficiently collect and transport the electrons produced by light absorption. Additionally, PCBM can function as a layer that blocks holes from reassembling into electrons, thereby enhancing effectiveness [9]. The bulk of heterojunction photovoltaic cells, which exhibit impressive efficiency juxtaposed with standard solar cells, are made up of PEDOT: PSS with PCBM.

Proposed analysis

Conventional solar panels made from perovskite frequently include lead, nonetheless due to safety and environmental issues, researchers have been looking for alternatives for replacing lead within these cells. A mixture of an organic–inorganic free of lead perovskite structure, which could be methylammonium tin triiodide or for mamidinium tin triiodide, constitutes one of the most intriguing options. These substances resemble lead-based perovskites in terms of physicochemical capabilities, but they don't include lead, thereby rendering them less dangerous and more ecologically friendly. Using non-toxic cesium-based perovskite photovoltaic cells is yet another possibility; cesium lead bromide ($CsPbBr_3$) is one such material. Fortunately, it comes with an inferior open-circuit voltage and a lower absorbance coefficient. Furthermore, extra substitute materials have been investigated as possible substitutes for lead in solar cells made from perovskite, including copper- and bismuth-based solar cells made from perovskite [10]. It ought to be emphasized that lead replacement for perovskite solar cells continues to be a hot area of study and that these new materials' stability and efficiency are continually being developed and improved. In a perovskite solar cell, PEDOT: PSS that has been doped by perovskite can be employed as a hole transport layer. a combination of their excellent performance and cheap cost, perovskite solar cells—a more contemporary form of solar cell—have shown considerable promise in recent years. PEDOT:

PSS has excellent electrical conductivity therefore order and it can efficiently transport holes created by the uptake of electromagnetic radiation within the perovskite layer, making it a promising hole transport semiconductor for perovskite solar energy cells. The perovskite photovoltaic cell's structural integrity may be enhanced by the PEDOT: PSS layer. Compared to classic solar panels and perovskite solar cells, hybrid solar cells—which combine PEDOT: PSS and perovskite—have a high efficiency. Graphene-doped PEDOT: PSS can be utilized as a layer that transports holes in solar cells. PEDOT: PSS's performance can be improved by using graphene, a single sheet of carbon atoms organized in a lattice that is hexagonal in shape. The addition of graphene fragments to PEDOT: PSS can make the PEDOT: PSS layer more conductive, which boosts the extraction and delivery of holes (either positively charged carriers) produced by the light absorption and boosts the solar cell's overall effectiveness. The increased surface area of graphene can also aid in enhancing and improving the quantity of PEDOT: PSS that can be included in the photovoltaic cell, resulting in more effective charge transfer. When compared to conventional solar cells that use PEDOT: PSS photovoltaic panels, hybrid solar cells—which combine PEDOT: PSS with graphene—have a high efficiency [11].

2 Materials and Methods

2.1 Mathematical Model

Recombination of charge-carrying particles (holes and electrons) in a material made from semiconductors is described theoretically by the Langevin recombination equation. Subsequently relies entirely on the Langevin hypothesis regarding carrier recombination, which posits that the square root of the carrier concentration determines the recombination rate of carriers. The Langevin recombination machine learning model's computational formula can be obtained by:

$$J = B * \mathrm{sqrt}(p * n) \tag{1}$$

In cases in which p is the hole-focused attention, n is the electron-focused attention, B is a constant that's designated to represent the Langevin recombination coefficient for beta absorption, and J is the coefficient of recombination current density [12]. Recombine in actual substances is typically more complicated and can require additional processes, such as Shockley–Read–Hall recombination, hence it should be emphasized that the Langevin recombination framework is an idealized model and cannot be applied to all semiconductors. Learning about the recombination process of carriers for semiconductors particularly plays a key role in determining the effectiveness of photovoltaic cells as well as various electronic components, is possible using the Langevin recombination paradigm [13].

2.2 Shunt Resistance

The obstacle caused by electrical flow in a photovoltaic cell which "shorts" the electrical connection connecting the cell's front and rear ends is measured. The shunt is a conducting route that permits current to flow across the photovoltaic cell's productive region, decreasing the cell's efficiency. Shunting resistance in a thin-film solar panel is brought on by flaws or imperfections in the semiconductor substance that provide a connecting route between both the front and back of the cell. These flaws might be microscopic fractures, vacancies, or other structural flaws that permit current to skip the cell's active region and lower the amount of current the cell generates [14]. By passing a modest volt over the semiconductor device and detecting the resultant current, the resistance of the shunt may be determined. By reducing the quantity of material flaws, either through better manufacturing techniques or the use of higher-quality materials, the resistance to shunt movement can be decreased. The use of a coating that is anti-reflective on both the outer and inner surfaces of the cell can also aid with lowering shunt resistance by reducing light scattering, which may contribute to improving the quantity of light that gets taken in by the active region of the cell [15]. Shunt conductance is one of the elements that may impact a thin-film solar cell's overall performance, and lowering it can boost the cell's efficiency [16].

Series Resistance

Energy is a measurement of the amount of resistance to electrical flow that arises along the course of the current as it passes through the solar cell's active region. The interaction between the semiconductor and the metallic electrode and the impedance of the semiconductor substance is to blame [17]. Series resistance within a thin-film photovoltaic cell can be brought on by a variety of things, including a semiconductor that is of poor quality, electrodes that make poor contact with the semiconductor, and an uneven semiconductor layer. By applying a modest circuit across the structure of the cell and counting the resultant current, series resistance may be determined [18]. By employing top-notch semiconductor materials, improving the interaction that exists between the semiconductors as well as the electrodes as well as and lengthening the semiconductor layer, the series resistance may be decreased. Additionally, it is possible to lower the series resistance by utilizing advanced production processes like laser scription and laser doping. Series resistivity is one of the elements that influence a thin-film solar cell's overall performance and lowering it can boost the cell's efficiency [19].

Numerical Simulation Formula

$$Rn, p = \frac{qnp}{\in\in o}(\mu n(E) + \mu p(E)) \tag{2}$$

$$J = qv_n\mu_n\varepsilon + qv_p\mu_p\varepsilon \tag{3}$$

$$\mathrm{div}(\epsilon\Delta\psi)=-\rho \tag{4}$$

Table 1 Material parameters used in simulation tool

S. No.	Parameters	PEDOT: PSS	P3HT: PCBM	AL	MASNL3
1	Electron trap density [11, 20]	1e20	3.8e26	1e18	1e18
2	Hole trap density [13]	1e20	1.4e25	1.2	1.3
3	Electron mobility [10, 21]	1e−05	2.48e−07	4.5	4.17
4	Hole mobility [19]	1e−05	2.48e−07	10	6.5/10
5	Eg [22, 23]	1.3	1.1	1×10^{18}	1×10^{18}
6	Thickness [24, 25]	200 nm	220 nm	100 nm	50 nm

$$J_n = q v_n \mu_n \varepsilon + q D_n \tag{5}$$

$$J_p = q v_p \mu_p \varepsilon - q D_p \tag{6}$$

$$J_{\text{cond}} = J_n + J_p \tag{7}$$

The general durability of perovskite solar cells depends on the choice of stable and compatible Electron Transport Layers (ETL) and Hole Transport Layers (HTL). To replace traditional HTL and ETL options, researchers are constantly examining new substances with enhanced stability and efficacy. Improved film perovskite shape overall crystallization may be achieved by post-deposition techniques with the value of chemical design as well as thermal annealing which boosts stability and effectiveness. These processes enhance charge transmission and improve the perovskite layer's performance. Identification of stability problems and degradation pathways can be aided by carrying out comprehensive tests over time and faster aging studies. It is possible for academics to create focused tactics to successfully address stability issues through an awareness of their deterioration mechanisms (Table 1).

Structure

Figure 1 represents the schematic structure of the simulation design used to analyze efficiency. Here we take Al as the base layer, MASNL3 is a sandwich between the active layer PEDOT: PSS and P3HT: PCBM. In this structure, we take ITO with Glass for more accelerating velocity for light absorption. The height of the structure size is 870 nm.

3 Results and Discussion

The mathematical modeling of an intricate multilayered architecture made of Glass/ITO/PEDOT: PSS/$MASnl_3$/P3HT: PCBM/Al constitutes the focus of this study. The P3HT: PCBM has a wavelength of 220 nm. The IV characteristics, quantization

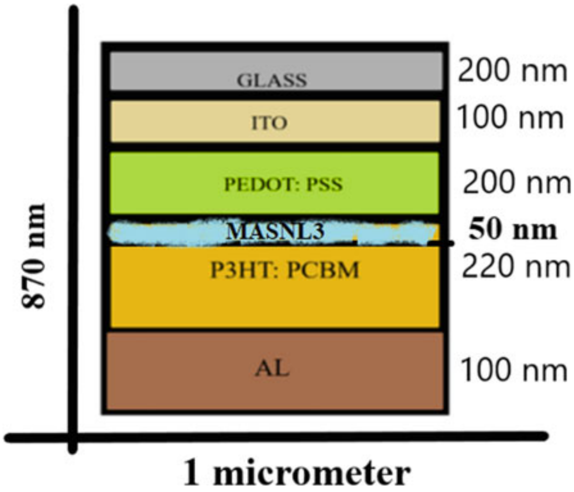

Fig. 1 IV characteristics Glass/ITO/PEDOT: PSS/ MAS_nl_3/P3HT: PCBM/Al

efficacy, and fill factor were all obtained. As is frequently observed, improving PCEs and raising Voc result from increasing dopant density. On the other hand, increasing the dopant thickness in the absorber part of HFRC and HFMC above cm-3 affects the recombination rate, which causes a drop in JSC.

3.1 IV Curve

We generated a 27.8% accuracy in Fig. 2. With the standard settings of SCAPS-1D software, we model the structure in 3 situations: first in AM1.5D, then in normal, and finally in under sun circumstances.

3.2 Quantum Efficiency

The line diagram in Fig. 3 above shows the efficiency of quantum systems as a function of wavelength. The fundamental structure of Glass/ITO/PEDOT: PSS/P3HT: PCBM/Al is used in the first study, and this was where we found the lower quantum conversion rate (Black), which was close to 56%. With the addition of $MASnl_3$ within the combination of PEDOT: PSS/P3HT: PCBM and normal conditions in the first circumstance, the second circumstance was explored. The graph's blue hue denotes the structure's 84% efficiency, which indicates an enormous growth in the quantum level. The 3rd scenario yielded 111.21% in quantum efficiency and has the same construction as the sun state, which is shown in blue.

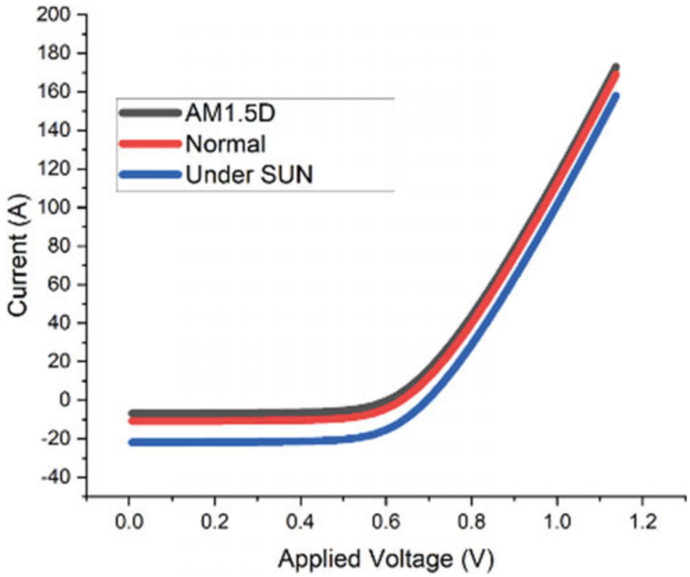

Fig. 2 IV curve current versus voltage

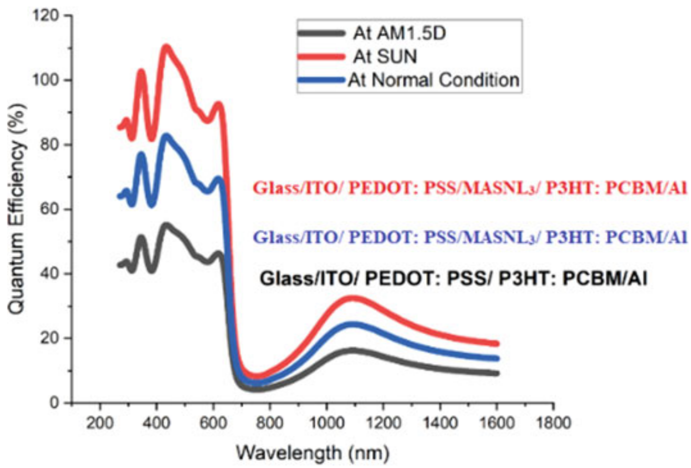

Fig. 3 Quantum efficiency versus wavelength (nm)

Generation rate

The emergence velocity of the electron in the layer that is active is shown in Fig. 4. In recent years, lead halide perovskites have shown tremendous promise as absorbent compounds for application in photovoltaic devices, demonstrating their broad potential. The materials have an astonishing 24.2% efficiency in converting energy.

Under sun condition

The plots in Fig. 5 show how the structure's absorption and electron dissipation. Since MASnl3 is very conductive, the electron may flow through it quickly.

Absorbed photon density

In Fig. 6 the graphs show the intensity of photon density absorption in the 250–650 nm.

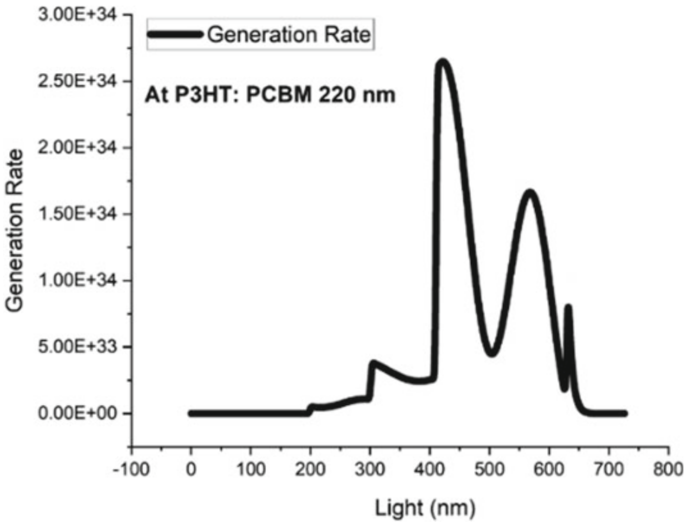

Fig. 4 Generation rate versus light (nm)

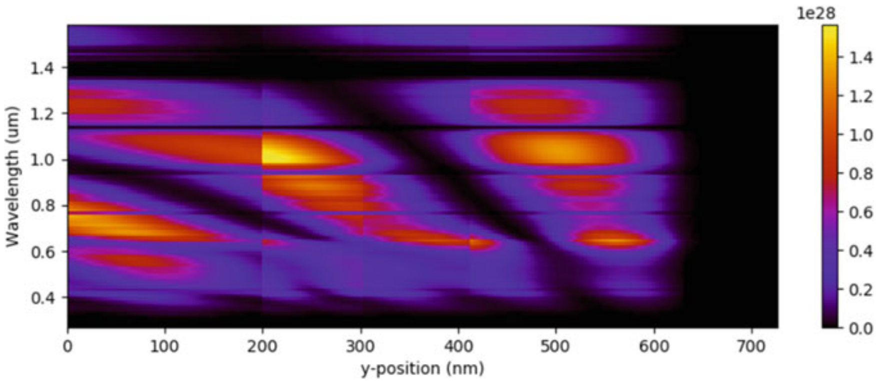

Fig. 5 Wavelength versus distance (nm)

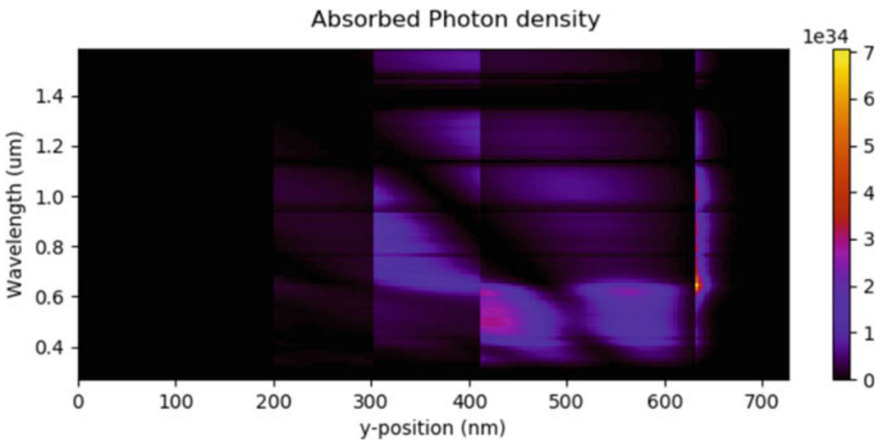

Fig. 6 Wavelength versus distance (nm)

4 Conclusion

In the end of the aim of this examination was achieved. A PCE efficiency of 27.8% was attained. When using Glass and ITO, the quantum efficiency rises to 110%. Three alternative scenarios were used for the analysis: AM1.5D, regular circumstances, and sun. The fill factor for the structure is 0.75. Furthermore, the point of origin photon's wavelengths and momentum are both improved by up to 500 nm, along with the internal translational efficacy.

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