The Performance of High-efficiency Perovskite Solar Cell (PSC) by Using Capacitance Simulator

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Abstract. Organic-inorganic perovskite-based solar cell fascinated researchers around the world with their immense interest. Since 2009, intensive work on photovoltaic perovskite systems reached efficiencies over 20% relative to silicon-based solar cells with a current efficiency of approximately 17%. The current research paper presents the suitable choice of solar cell materials such as hole transport materials, type of perovskite material, the electron transport layer among others. A photovoltaic device is then built using the chosen materials which are then investigated through simulations using the SCAPS 1D program to determine the effects that these layer materials have on the performance of the overall PV device. Simulation methods are also used to optimize the parameters of the constructed device such as the thickness of the electrodes, the hole transport layer and the light absorber material. The simulation results showed an efficiency of 20.34 % using gold (Au) contacts.

1. Introduction

Previously, the cells of silicon solar have had a reliability of just 12-17.5% for every PCE [1], that led to an extensive search for new materials to replace cells of silicon in order to improve efficiency [2]. As being such, researchers began to look into the photovoltaic technologies hybrid (organic-inorganic) materials. Hybrid photovoltaic is a state-of-the-art technology compared to inorganic solar cells (Silicon base) used as the primary material for solar cell production. An instance of a hybrid solar cells is the perovskite solar cells (PSCs), which since 2009 have received special attention with a dramatic increase in production from 3.8% to 23.3% comparison with the cells silicone solar [3]. Hybrid perovskite photovoltaics give a compelling combinations of high device performance and fabricating, ease of processing and enormously low-cost [1, 2].

A standard perovskite-based solar cell contains six large layers of different components. These are the gold electrode, hole transport layer, a perovskite material, an electron transport layer and glass transport electrode [1]. The composite of solar cell as the materials for hole (Spiro-Ometad, CuO, Cu2O), the type of perovskite material, the electron transport layer TiO2, among others.

The Hybrid (organic-inorganic) polycrystalline solar cells has electrical property of absorbing also the near-infrarot as compared to solar cell c-silicon (c-Si) that can only soak up the ultraviolet spectrum. Moreover, in about 9 years, the cells of perovskite solar have reached the 23 %, rendering it an outstanding candidate for silicon. The aim of this paper is then to optimize efficiency through
simulation. The Devices are illustrated by contrasting it to experimental data and using those parameters for optimal design study. We already discussed the effect of the defects on solar cell performance, doping concentrations and the active layer thickness [1].

2. Materials and Methods

Perovskite can be defined as any material with a similar crystal structure to the titanate mineral calcium (CaTiO3) at different transition state, see for example Fig. 1. ABX3 formula illustrates the perovskite crystal structure in which A is a powerful cation (inorganic or organic), B is a divalent tiny metallic cation such as Eu2+, Pb2+, Ge2+, Sn2+, Mg2+, Cu2+ and Yb2+, and X is the halide ion [6].

Figure 1: Many ABX3 compounds

This discovered (1990s) that halide was able to convert light-electricity and allowed it light-emitting diodes (LEDs). Perovskite form consists of four possible phases: α, β, γ and δ. On the one side, α is a process of T > 327 K with structure (e.g., CsSnI3). The process makes just one formula unit per cell. CH3NH3+ can’t shape the cubic structure at this temperature. On the other side, at T < 327 K, the perovskite transitions of β to α. The lattice parameters of α and c (8,855, 12,659) Å and the exact measurement of these lattice parameters depend on the molecular position. The tolerance factor is given by:

$$t = \frac{(R_A + R_X)}{\sqrt{2} (R_B + R_X)}$$

(1)
where, $R$ is the ion radius, and suffixes (A, B, X). To have a robust perovskite, Hendon et al. reported that the tolerance factor is $0.7 < T < 1$ [7]. Where cation A must be more important of B. One of the best options in this respect is CH$_3$NH$_3$ ion. If the factor of tolerance is high, a lower tetragonal symmetry ($\beta$-phase) or ($\gamma$-phase) orthorhombic symmetry may result. The conversion happens at 3270 and 160 K respectively from $\alpha$ to $\beta$ to $\gamma$. The transition of perovskite and rotation of the polyhedral BX$_6$ in lattice. While a non-perovskite process is the fourth step ($\chi$). ABX$_3$ (MAPbI$_3$) typically has a cubic and $\alpha$-phase configuration, B=6 closest, X ions (octahedral) and A has 12 fold coordinating sites (Figure 3) [8, 9].

Figure-3: Cubic structure (MAPbI$_3$)

"1s$^2$2s$^2$2p$^6$3s$^2$3p$^6$3d$^{10}$4s$^2$4p$^6$4d$^{10}$4f$^{14}$5s$^2$5p$^6$5d$^{10}$6s$^2$6p$^2$ is the electronic configuration of lead (Pb). The 6s orbital is occupied, which is beneath the top of the HUMO band of the perovskite material. LUMO is derived virtually of p orbit of Pb, unlike GaAs and CdTe. Furthermore, due to the nature of the electronic structure, perovskite gets covalent and ionic. Moreover, the organic (CH$_3$NH$_3$+) have not effect to measure the electronic performances but participates in changing the lattice constants and stabilizing the perovskite phase structure, instead. MAPbI$_3$ perovskite has a various electronic structure in comparison to the traditional semiconductor. In addition, HOMO is also dispersive as a result of the robustness of s-p coupling" [6, 7].

The effective electron mass ($m^*$) well-adjusted by the effective hole mass ($h^*$) in MAPbI$_3$ perovskites that ultimately leads to an aggressive charging behavior in hybrid solar cells can be provided by the relationship [8]:

$$m^* = h^2 \left[ \frac{\partial^2 \epsilon(k)}{\partial^2 \kappa} \right]^{-1}$$

(2)

It is important to mention that the light absorber material is the heart of the photovoltaic solar cells and it is crucial in achieving excellent performance. Therefore, the optical absorption coefficient and size are the critical factors of the products that absorb light. The edge transformation for MAPbI$_3$ perovskite comes from a combination of Pb s-p coupling and p orbital so there is a significant chance of change from Pb to Pb. Perovskite is a clear bandgap substrate and therefore has significant absorption intensity and a wider range to solar energy beyond the visible spectrum to achieve high power output values. Solar Cell (PSC) output relies primarily on the absorption intensity [5,6]. First, the point defects, which are consist of two types of Schottky and Frenkel inside the intrinsic material and the grain-boundary [8], which significantly influence the diffusion length of the electron and hole (L$_n$, L$_p$, respectively) and open circuit voltage (VOC) of cell. Second, the crystalline structure of light-absorbing material [9]. The density of the defect of the hybrid perovskite layer rely upon the creation of energy and therefore, the chemical potential of the organic-inorganic mixture. The low formation energy defects are better due to the creation of shallow level of defects, a result that is required to have a long diffusion length of the electron-hole and a high open-circuit voltage (VOC). In the current study, a considerable understanding will be obtained regarding the energy level of different
layers of the Solar cell, as degree of level of the mixture determines the energy gap of each layer and its position in the final stage of the device fabrication. Therefore, the simulation outcomes of the long diffusion length of the electron-hole and the high open circuit voltage will be in the accordance with the shallow defect levels [8,9].

“p-type doping in copper indium gallium selenide (CIGS) with the chemical formula (CuInxGa(1-x)Se2) and in cadmium telluride (CdTe) is easier than n-type doping. This is because of the self-compensation in equilibrium. Both semiconductors are of direct bandgap, in which the electrons travel directly from (VB) to (CB) without losing any energy. This can absorb the light in a much thinner area. Therefore, it can be produce with a skinny active layer of a thickness of less than 1 μ. In a sense, it is possible to use the above comparisons to the silicon doping procedures to produce a material of n-type and p-type, in which an impurity atom from group 5 will produce n-type (donor like) and group 3 will produce p-type (acceptor-like) semiconductors. The robustness of the covalent bonds and the deep level defects can be measured by the calculations [6,7,9]. Therefore, doping either n-type or p-type in the Hybrid perovskite (organic-inorganic material). Thus, the main aim of this research paper is to investigate the n and p doping in this Hybrid materials”.

The power conversion efficiency (PCE) of cell increased quickly in comparison to Si solar cell over the years as shown in Fig. 4 [9].

Figure-4: Comparison of the Silicon and Perovskite efficiencies over the years [9]

The comparison makes a strong choice for the perovskite. The purpose of manufacturing a solar photovoltaic cell is to maximize the cost-to-cost Power Conversion Efficiency (PCE). In fact, the perovskite class is MAPbBr3, MAPbCl3 and MAPbI3 as a consequence of this rapid improvement of the hybrid (organic-inorganic) material nature. MAPbI3 is one has proven to be strongest perovskite because of its significant electrical and optical properties. Process ability of low-temperature solutions, long service life and ferroelectric strength. The performance of cell improved not only to the absorber but also to all layers by means of different design techniques (See Fig. 5) [10].
Simulation is a good choice for observing the actual process, the feasibility of a given physical model, as well as of knowing the function of device and design parameter influence real activity and output of cell systems immediately without having money before seeing the results [10]. Throughout the photovoltaics technologies a range of simulation models were used, such as TCAD, SILVACO, SCAPS, GPVDM, COMSOL MULTIPHYSICS and AMPS. In this research Solar Cell Capacitance Simulation (SCAPS) simulation was used to cells of perovskite. It may describe up to seven layers of semiconductors. Additionally, SCAPS 1D has a very random period of activity and diversified models for scoring, mutations, recombination and generation. Once it has established all the criteria, it functions like a real-life equivalent. Together with MATLAB simulator, this simulator (SCAPS) used to simulate the cells. The differential equations were applied in one dimension (1D) [10,11]:

\[
\begin{align}
\frac{\partial^2 \varphi}{\partial x^2} &= \frac{q}{\varepsilon} \left[ n(x) - p(x) - N_D^+(x) + N_A^-(x) - n(x) + p(x) \right] \\
I_{n,p} &= n q \mu_n E + q D_n \frac{\partial n}{\partial x} + p q \mu_p E - q D_p \frac{\partial p}{\partial x} \\
L_{n,p} &= \left( \frac{K_n^T}{q} \right) \mu_{n,p} \\
D_{n,p} &= \left( \frac{K_n^T}{q} \right) \mu_{n,p} \\
\frac{\partial n}{\partial t} &= \frac{1}{q} \frac{\partial}{\partial x} \left[ G_n - R_{n,+} \frac{1}{q} \frac{\partial p}{\partial x} + (G_p - R_p) \right]
\end{align}
\]

Where \( \varphi \) = electrostatic potential, \( q \) = elementary charge, \( \varepsilon \) = permittivity, \( n \) = density of electron, \( p \) = density of hole, \( N_D^+ \) = ionized donor, \( N_A^- \) = ionized acceptor, \( p_t \) = trapped hole density, \( n_e \) = electron density, \( L_{n,p} \) = diffusion length (electron, holes), \( D_{n,p} \) = electron and hole diffusivity, \( \mu_n \) = electron mobility, \( \tau_n \) = electron lifetime, \( n-p \) is the electron-hole concentration, \( E \) = electric field, \( \frac{\partial n}{\partial x} \) = concentration gradient (electrons-holes), \( G_{n,p} \) = optical generation rate, and \( R_{n,p} \) = recombination rate.

In the simulation, Perovskite Solar Cell (PSC) was used in a solid state planar heterojunction structure n-i-p with intrinsic perovskite material sandwiched used as the material conveying the hole (HTM). SnO2: F is the conductive transparent oxide (TCO) and gold as a conductor (Fig. 6). As one of frequently used simulators in cell. SCAPS is used to test PSC[10]. It is a one-dimensional (1D) simulation system for solar cells focused on the three central differential equations of Poisson's theorem, equation of transport, and equation of continuity. This section is divided into two sub-sections as mentioned in details in below.

Solar Cell Capacity Simulation (SCAPS) was used to determine the efficiency of the system. The design of the cells can be seen in Figure 7. The variables used throughout the simulation were chosen from
different discourses. The parameters were taken from the normal meaning for the cavity conveying content and the absorber layer. Fig. 8 shows the band diagram of the cell. By this figure the absorber will consume sunlight for a lower bandgap. In this way, free electrons and holes formed, resulting in more current, i.e. improved filling factor [10,11].

Table 1 shows device parameter used to model electrical and optical properties from HTM and TCO literature. TiO$_2$[12] was used as a blocking layer here. NA and ND represent the acceptor and donor concentration, respectively. $\epsilon_r$ is permittivity, $E_g$ is the energy gap, $\chi$ is the electron affinity, $\mu_n$ and $\mu_p$ represent the electron and hole mobility, respectively [13]. Therefore, the layer is almost intrinsic type. The defect type is neutral and energetic distribution is single and Gaussian has a characteristic value of 0.1 eV. Cross-section area of electron and hole is choosen to be 2×10-14 cm$^2$. The simulation is then performed under AM1.5 G at 300 K [11-13].

Table-1: Parameters of Solar Cell

| Parameters                      | SnO$_2$:F | TiO$_2$ | CH$_3$NH$_3$PBI$_3$ | Spiro-OMeTAD |
|--------------------------------|-----------|---------|--------------------|--------------|
| VB effective density of states (1/cm$^3$) | 2.20E+16  | 1.80E+19 | 1.00E+18 | 1.80E+19 |
| electron affinity (eV) $\chi$ | 4         | 4.26    | 3.9               | 2.2          |
| CB effective density of states (1/cm$^3$) | 2.20E+17 | 2.00E+18 | 2.20E+18 | 2.50E+18 |
| hole thermal velocity (cm/s) | 1.00E+07  | 1.00E+07 | 1.00E+07 | 1.00E+07 |
| electron thermal velocity (cm/s) | 1.00E+07 | 1.00E+07 | 1.00E+07 | 1.00E+07 |
| hole mobility (cm$^2$/Vs) | 1.00E+01  | 1.00E+03 | 2.20E+00 | 2.00E-04 |
| electron mobility (cm$^2$/Vs) | 2.00E+01  | 2.00E+04 | 2.20E+00 | 2.00E-04 |
| Thickness (nm) | 500       | 100     | 50-600            | 300          |
| shallow uniform donor density ND (1/cm$^3$) | 1.00E+15 | 6.00E+19 | 9.00E+20 | 0.00E+00 |
| dielectric permittivity $\epsilon_r$ | 9         | 38-108  | 30                | 3            |
| bandgap (eV) $E_g$ | 3.5       | 3.2     | 1.55              | 2.9          |
| shallow uniform acceptor density NA (1/cm$^3$) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 1.00E+22 |
| N$_T$ Total (cm$^{-3}$) | 1.00E+15 | 1.00E+15 | 8.50E+13 | 1.00E+15 |
| Contacts (Au) | Work function (5.1 eV) |
Figure-6: SCAPS-1D Solar definition panel with PSC cell layers name

Figure-7: SCAPS-1D Solar definition panel

Figure 8 shows the SCAPS definition panel. It consists of 7 layers defined with different parameters and materials.

Figure-8: The simulation results of PSC for Au contact

3. Results and discussion

One of the most critical parameters, which has a considerable effect on the device performance is the thickness of the perovskite absorber layer (50-600) nm. In this simulation, we concentrate on the most important electrical properties parameters of the cell of Jsc, Voc, and short-circuit current density. The default parameters for layers as shown in Table 1. Our findings indicate that as the thickness increase, Jsc also increases and reaches the maximum value of around 15.158 mA/cm² at about 300 nm, followed by a slight decrease. VOC increases to an optimal value at 200 nm and decreases afterward. In addition, filling factor grows when thickness increases. The efficiency similar to Voc, as it increases to an optimal value (300 and 400) nm, and then decreases with the thickness keeps growing. When the absorber is thin, the length of the charge carrier diffusion is longer from width and the majority of the excess carriers can
reach the electrodes to produce power. An increase in the depth, on the other hand results in further light absorption and excess carrier concentration. Which makes Jsc to be at the elevate. Due to the fact that the perovskite material has extremely high absorption coefficient, which is usually up to 105 cm\(^{-1}\), the cell can obtain extremely high amounts of Jsc and PCE for absorber. 

VOC can then be defined by the formula [15,16]:

\[ V_{OC} = \frac{n k B T}{q} \ln \left( \frac{I_L}{I_0} + 1 \right) \]  

(8)

Where \( n \) is factor, \( k B T/q \) = thermal voltage, \( I_L \) = light that produce current and \( I_0 \) = dark saturation current. Filling factor, on the other hand can be considered as the ability of delivering the available power to a load among the maximum power produced by a cell, when the thickness is less than 500 nm.

As the thickness rises to some degrees, the PCE decreases and the internal power loss increases above 300 nm, too. Moreover, the declining influence of the PCE will be observed at a thickness of more than 300 nm, which will be attributed to more recombination due to the increase in the amount of traps and also due to the increasing number of excess carriers that cannot enter the electrodes. Thicker absorber, in this situation, causes declines in PCE and Voc. Two variables in photon absorption and carrier distribution influence the efficiency of the solar cell in the current simulation. While the former factor is the thin absorber determinant, the latter factor is the dense absorber determinant. It can be found that the ideal thickness at 300 nm would equate to the optimal value of the PCE.

4. Conclusions

In simulating perovskite solar cells, we utilized the device simulator SCAPS 1D. For inorganic solar cells SCAPS-1D simulator is commonly used. We have already used TiO2 materials throughout this study, which also exhibits quite similar characteristics to ZnO. Use TiO2 as the electron transport layer and gold as a touch layer to achieve a high performance of 20.34 % with FF of 90.1 % shows better consistency as transportation fiber. The simulator results of solar cell may support for improving in organic cell efficiency. It is examined influence of absorber thickness on perovskite cell such as \( \eta \), FF, JSC and VOC. The study of our results indicated the importance of the thickness of the contact layer and the absorber thickness for optimal performance.

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