Simulation and analysis of schottky junction perovskite solar cells (SJPSCs)

Numeshwar Kumar Sinha1*, Priyanka Roy1, Dhriti Sundar Ghosh2 and Ayush Khare1

1Thin Film Research Laboratory, Department of Physics, National Institute of Technology, Raipur – 492 010, India
2Department of Physics, Indian Institute of Technology, Bhilai, GEC Campus, Sejbahar, Raipur – 492 015, India

*Corresponding author’s e-mail address: nksinha.phd2018.phy@nitrr.ac.in

Abstract. The Schottky junction solar cells are the simplest and single-layer structure of solar cells, offering low-cost and easy fabrication. In this study, we have simulated and analyzed the Schottky junction perovskite solar cells, having the device structure of FTO/MAPbI3/Au. The simulation has done by Solar Cell Capacitance Simulator (SCAPS-1D). In this simulation, we have studied the effect of an absorber layer thickness, doping density, defect density, and the cell’s temperature on the performance of the cells. We have further studied the effect of different back electrodes, like Au, Cu, Ag, Al, and Graphene in the performance of cells. The effect of series and shunt resistance has also been studied at optimized parameters. This simulation suggests that the SJPSCs show the highest optimized power conversion efficiency of greater than 14%, at actual series and shunt resistance of the cell. Simulating this simplest structure will help to further improvement in the performance of SJPSC. However, the use of lead makes the solar cells non-eco-friendly, but the proper encapsulation and disposal management can solve this problem.

1. Introduction
The Perovskite material, which is used for making solar cell devices, has properties that, it has high carrier mobility [1], long diffusion length [2], high charge carrier lifetime[3], high absorption coefficient [4] and tunable bandgap [5]. The Perovskite Solar Cells can be processed by solvent engineering techniques, which provide wide varieties of cheap fabrication methods, like spin coating, dip coating, screen printing, etc. [6]. Due to such properties and easy fabrication techniques, the perovskite solar cells have been taken great interest and in just one decade the efficiency of PSCs has been accomplished to 25.5%, which very close to commercially available c-Si solar cells [7]. A Schottky junction solar cells are the metal-semiconductor interface, which offers, hand, bending energy band diagram and that separates light generated carrier towards the electrodes. The Schottky junction solar cells (SJSCs) show their maximum performance when one contact is Ohmic and the other is barrier contact. The SJSCs are the simplest solar cells and beneficial for further reduction in the cost of solar cells. To form a Schottky barrier, the work function of the metal should be higher as compared to the electron affinity of the semiconductor for the case of n-type semiconductor, but for the p-type semiconductor, the work function of metal should be small. In our case, we have used the n-type CH3NH3PbI3 (MAPbI3) absorber layer,
having an electron affinity of 3.9eV, with high work function metals [8]. In the present study, we have simulated SJPSCs with help of the Solar Cell Capacitance Simulator (SCAPS-1D)[9] and studied the effect of absorber thickness, doping density, defect density, and cell temperature on the performance of the cell. We have optimized all these parameters. The effect of different back electrodes and effect of series and shunt have also been studied. Our study reveals that, Au back electrode shows the maximum efficiency and Al is not suitable for the making of SJPSCs. Graphene, an interesting two-dimensional structure, has drawn intense interest due to its high stability, great charge carrier mobility and excellent conductivity[10][11]. In our simulation, we have used graphene layer as an electrode and achieved the efficiency of 14.14%. The use of graphene electrode can be suitable for further cost reduction of the device. We have achieved the optimized efficiency of 14.48% at series and shunt resistance of 3.18 Ω.cm$^2$ and 758 Ω.cm$^2$ respectively for FTO/n-type MAPbI3/Au structure.

2. Methodology and Simulation Parameters
For a simulation of the device, we have used SCAPS-1D simulation package, which is a one-dimension solar cell simulation program developed by the Department of Electronics and Information System, University of Gent, Belgium[12]. It is a completely computer-based software tool and adapted for analysis of homojunction, heterojunction, multi-junction, and Schottky junction solar cells. SCAPS is based on solving the one-dimension Poisson’s equation,

$$\frac{\partial^2 \varphi}{\partial x^2} = \frac{q}{\epsilon} [n(x) - p(x) - N_d^+ (x) + N_a^- (x) - P_t^+ (x) + N_e^- (x)]$$

and continuity equation of electrons and holes.

$$\frac{\partial n}{\partial t} = \frac{1}{q} \frac{\partial J_n}{\partial x} + G - R$$
$$\frac{\partial p}{\partial t} = - \frac{1}{q} \frac{\partial J_p}{\partial x} + G - R$$

Here, $\varphi$ is the potential, $q$ is the elementary charge, $\epsilon$ is the permittivity, $n$ is the density of free electron, $p$ is the density of free holes, $N_d^+$ is the ionized donor like doping density, $N_a^-$ is the ionized acceptor like doping density, $P_t^+$ is trapped hole density, $N_e^-$ is trapped electron density, $R$ is the recombination rate, $G$ is the generation rate, $J_n$ is current density due to electrons, $J_p$ is current density due to holes.

The simulation parameters of different layers, chosen very carefully form different research, are given in table 1[13–15]. The simulated device structure is shown in figure 1(a) and the band diagram is shown in figure 1(b). In this SCAPS-1D simulation package, we can add up to seven layers. In such simulation packages, initial conditions are very important to find the exact solution. In the equilibrium state, where there is no light and no voltage applied, initial conditions are taken into account by assuming that the quasi-Fermi level in the system is at zero and no conceivable drops throughout the structure. The short circuit current density is determined as calculation begins after illumination and this is set to be the next initial guess. Layer by layer, this process continues and obtained the final optimized solution.
Table 1. Simulation Parameters of different layers used in the simulation.

| Parameters                          | MAPbI$_3$         | Graphene | FTO  |
|-------------------------------------|-------------------|----------|------|
| Thickness ($\mu$m)                  | 0.1 – 1.2         | 0.05     | 0.05 |
| Band-gap (eV)                       | 1.5               | 0.8      | 3.5  |
| Electron Affinity (eV)              | 3.9               | 4.8      | 4.4  |
| Dielectric Permittivity (Relative)  | 30                | 7.1      | 9    |
| CB effective density of states (cm$^{-3}$) | 2.5x10$^{19}$  | 3x10$^{19}$ | 2x10$^{18}$ |
| VB effective density of states (cm$^{-3}$) | 2.5x10$^{19}$  | 3x10$^{19}$ | 2x10$^{18}$ |
| Electron Thermal velocity (cm/s)    | 1x10$^7$          | 1x10$^7$ | 1x10$^7$ |
| Hole Thermal Velocity (cm/s)        | 1x10$^7$          | 1x10$^7$ | 1x10$^7$ |
| Electron Mobility (cm$^2$/Vs)       | 15                | 1x10$^1$ | 2x10$^3$ |
| Hole Mobility (cm$^2$/Vs)           | 15                | 1x10$^5$ | 2x10$^3$ |
| Donor density (cm$^{-3}$)            | 1x10$^{13}$ – 1x10$^{16}$ | 00      | 2x10$^{19}$ |
| Acceptor Density (cm$^{-3}$)         | 00                | 1x10$^{16}$ | 00   |

Figure 1. (a) Structure of simulated device and (b) band diagram of the device.

3. Results and Discussions

3.1. Effect of absorber thickness on the performance of the cells

The performance of the cell varies with the thickness of an absorber layer as shown in figure 1. We have varied the thickness of an n-doped CH$_3$NH$_3$PbI$_3$ (MAPbI$_3$) from 0.1 $\mu$m to 1.2 $\mu$m. As increasing the thickness, the short circuit current density ($J_{sc}$) and open-circuit voltage ($V_{oc}$) increases as shown in the figure 2, it may be due to increasing the total number of electron-hole pairs as increasing the thickness[16]. The efficiency of the cell increases with increasing the thickness of an absorber layer and reached to optimum value at 0.75 $\mu$m. Further increasing the thickness, $J_{sc}$ of the cell get saturated and it may be due to increasing the collection probability of light-generated charge carriers by the junction[17][18]. The $V_{oc}$ of the cell decreases, caused by the increase in the recombination as increasing the thickness, and thus the overall performance decreases[15]. For larger the lifetime of the charge carrier will increase the efficiency of the cell at a particular thickness of an absorber layer[19].
3.2 Effect of doping density of an absorber layer on the performance of the cells

MAPbI$_3$ has properties that it can behave like n-type or p-type depending on the ratio of MAI/PbI$_2$[20]. Experimentally, it has been found that, if the film is MAI rich then it behaves as p-type whereas if the film is PbI$_2$ rich then the film work as n-type[21][22]. In our simulation, we have used an n-type MAPbI$_3$ perovskite material. We have studied the effect of an n-type doping concentration of an absorber layer on the performance of the cells by varying the doping density from $10^{13}$ cm$^{-3}$ to $10^{18}$ cm$^{-3}$. Increasing the n-type doping concentration increases the Fill factor (FF) and $J_{sc}$ of the cell because increasing the doping concentration increases the conductivity of the materials and increases collection of the light-generated charge carriers[23]. From Quantum Efficiency (QE) figure 4 (a), it clear that the charge collection slightly increases with increasing the doping density and but for larger the doping density QE get reduces. The increasing the doping density also increases the defect in the material which increases the recombination of the material[22]. As from figure 4 (b), it clear that the recombination rate in the material increases very when we increase the doping concentration from $10^{16}$ to $10^{18}$ cm$^{-3}$. That leads to decreasing in the $V_{oc}$. The overall efficiency of the device remains approximately the same for doping density $10^{13}$ to $10^{15}$ cm$^{-3}$ and decreases rapidly after doping density increases from $10^{15}$ to $10^{16}$ cm$^{-3}$.

![Figure 2](image1.png)  
**Figure 2.** Effect of an absorber thickness on the performance parameters of the device.

![Figure 3](image2.png)  
**Figure 3.** Effect of doping density of an absorber layer on performance parameters of the device.
3.3. Effect of defect density of an absorber layer on the performance of the cells

The defects in the solar cell’s material play a very important role. The defects create an intermediate energy level between the conduction band and valance band and work as a recombination center [24][25]. Thus, increasing the defects in the material will increase the recombination[26]. The defect reduces the diffusion length and lifetime of the charge carrier and thus reducing the collection probability of light generated carrier by the junction[27]. As we increase the defect density in the light-harvesting material from $10^{13}$ to $10^{15}$ cm$^{-3}$, all the performance parameters get reduces tardily but when we further increase the defect density from $10^{16}$ to $10^{18}$ cm$^{-3}$ the performance parameters get reduces linearly approximately.

3.4. Effect of cell’s temperature on the performance of the cells

In India, at different seasons, the various regions have different temperatures[28] and the analysis of the influence of the temperature of the cells becomes more significant. The temperature of the cell has been varied from 300K to 350K. The increase in the temperature increases the recombination current or dark current and thus decreases the $V_{oc}$ of the device[29]. Increasing the temperature decreases the energy gap of the material by increasing the thermal energy of the charge carriers with temperature[30] and that leads to increasing the $J_{sc}$ as temperature[31] as shown in the figure 6. From the figure 6, it is clear that the rate of increasing of $J_{sc}$ is very small as compared to the rate decreasing of $V_{oc}$, thus the overall efficiency of the cell decreases with increasing the cell’s temperature.

3.5. Effect of series and shunt resistance

The series resistance comprises resistance of all the layers in the device whereas, shunt resistance is due to defects and poor quality of the cell. The series resistance predominately affects the $J_{sc}$ and Shunt resistance mainly impacts $V_{oc}$. The effect of series and shunt resistance on the cell’s performance at optimized parameters (Thickness = 0.75μm, $N_D = 10^{15}$ cm$^{-3}$, $N_I = 10^{13}$ cm$^{-3}$, Temperature 300K) has been studied. The cell shows 16.98% efficiency by considering the cell as an ideal solar cell in which there is no series and shunt resistance. But in the actual device, the series and shunt resistance must present, and when including the series and shunt resistance the device shows 14.48% efficiency for series and shunt resistance of 3.15Ωcm$^2$ and 758Ωcm$^2$ respectively. These values of series and shunt resistance are corresponding to the actual device which we have taken from the experiment of another researcher[32].
Figure 5. Effect of defect density of an absorber layer on the performance parameters of the device.

Figure 6. Effect of cell temperature on the performance of the cell.

Figure 7. J-V curve of the cell for (a) an ideal case and (b) due to effect of series and shunt resistance.

3.6. Effect of different back electrodes
The built-in-potential ($V_{bi}$) plays a vital role in the performance of solar cells. The built-in-potential provides the necessary action of separation of light-generated charge carriers. In the Schottky junction solar cells, the built-in-potential is defined as [22] in equation (3).
Where, $E_C$ is conduction band of n-type perovskite, $E_F$ is the fermi level of n-type semiconductor, $q$ is an electronic charge, and $\Phi_B$ is Schottky barrier height at metal/perovskite interface defined as

$$
\Phi_B = \Phi_m - \chi
$$

Here, $\Phi_m$ is the work function of metal and $\chi$ is the electron affinity of semiconductors. From equation (3), it is clear that the built-in-potential strongly depends on the work function of the metal. When we move from high work function back electrode to low work function back electrode, the strength of $V_{bi}$ decreases and thus decreasing the overall performance of the cells as shown in table 2. The device shows the maximum efficiency of 14.48% for the case of Au back electrode. For the case of Al back electrode, our device does not work. It may be due to a lower strength of $V_{bi}$, that might not sufficient to separate the light-generated charge carriers towards the electrode to generate the photovoltaic effect.

The graphene has high conductivity[33] and high charge carrier mobility[34] and forms a Schottky junction between graphene/perovskite interface because of its high work function[35]. In our simulation, by adding a graphene layer above the perovskite layer, as parameters given in table 1, the device shows 14.14% efficiency. The use of graphene may be a good alternative of Au for making highly efficient SJPSCs and for further diminution of the cost of the cells.

### Table 2. Effect of different back electrodes on the performance parameters of the device.

| Device Structure          | $V_{oc}$ (V) | $J_{sc}$ (mA/cm$^2$) | FF (%) | Efficiency (%) |
|---------------------------|--------------|----------------------|--------|----------------|
| FTO/MAPbI$_3$/Au          | 0.815726     | 27.08188             | 65.5365| 14.4779        |
| FTO/MAPbI$_3$/Graphene    | 0.760943     | 25.62309             | 72.5078| 14.1374        |
| FTO/MAPbI$_3$/Cu          | 0.430565     | 26.97764             | 45.6396| 5.3013         |
| FTO/MAPbI$_3$/Ag          | 0.232208     | 24.85145             | 28.3431| 1.6356         |
| FTO/MAPbI$_3$/Al          |              | Cell do not work     |        |                |

### 4. Conclusions

In this study, we have simulated SJPSCs by using SCAPS-1D simulation package. our simulated device structure is FTO/n-type MAPbI$_3$/back electrode. We have simulated and analyzed the effect of absorber’s thickness, doping density, defect density, and cell temperature on the performance of the device and optimized all these parameters. The device shows the efficiency of 16.98% for the case of ideal solar cells and when we include the effect of series and shunt resistance, the device shows the efficiency of 14.48% at series and shunt resistance of 3.18 $\Omega$.cm$^2$ and 758 $\Omega$.cm$^2$ respectively. The effect of back electrodes has also been studied. The device shows a maximum efficiency of 14.48% for FTO/n-type_MAPbI$_3$/Au structure. Our simulation suggests that Al is not suitable for the making of SJPSCs because of its low work function. By using graphene as an electrode, we obtained an efficiency of 14.14% and maybe the promising alternative of gold.

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