

Simulation of Perovskite Based Solar Cell Using SCAPS Software

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Abstract

In this paper, a simulation of perovskite based solar cell and an analysis on the performance parameter like effect of temperature and effect of thickness of absorber is carried out. The absorber material as well as the perovskite material is taken as $\text{CH}_3\text{NH}_3\text{PbI}_x\text{Br}_{1-x}$. The performance parameters are compared in terms of efficiency, open circuit voltage, short circuit current and fill factor. It is found that as temperature increases, the efficiency of this solar cell decreases and as thickness of absorber layer increases the efficiency is increased up to 23.16% at 500 nm. The simulation is carried out in SCAPS version 3.3.07.

Keywords

Perovskite, Solar cell, Absorber, Nano

Introduction

Traditionally, the energy from fossil fuel sources is insufficient to support the sustainable growth of human society. Using clean, renewable sources of energy has come to be seen as essential to the advancement of human life. Solar power is probably one of the most highly promising energy options out of the many available [1]. A solar cell is a device that uses photovoltaic effects to transform light energy directly into electrical energy. Typically, silicon has been used to make solar cells, but due to the large size and high cost of manufacturing it is replaced by another type of material known as Perovskite material, that has an excellent absorption coefficient [2], high transport properties, carrier or charge mobilities that results in a high efficiency device. There are mainly five fundamental layers for a perovskite solar cell, an absorber or perovskite material, electron transport layer (ETL), hole transport layer (HTL), transparent conductive layer, and a metal electrode. The perovskite material is placed between the ETL and HTL.

The perovskite can be represented in the form of ABX_3 where A is an organic cation like methylammonium, or it can be formamidinium. The methylammonium can be represented by CH_3NH_3^+ and formamidinium by $\text{NH}_2\text{CHNH}_2^+$. The letter B indicates an inorganic cation mainly lead(II) which is represented by Pb^{2+} . The letter X_3 is a small halogen anion typically neither chloride nor iodide [3]. Here the hole transport material is taken as NiO_x which is a p-type material and electron transport material is taken as ZnO_2 which is a n-type material. The most widely used metal oxide in solar cell structure is ZnO because of having high conductivity, high electron mobility, low cost and high resistance to photo corrosion.

Enhancing the electrical and optical properties of perovskite solar cells can be achieved effectively by integrating a polymer nanocomposite, particularly P3HT polymer gold nanoparticle, as the HTL that leads to improved photon

absorption efficiency. Utilizing this polymer nanocomposite in the production of perovskite solar cells can result in the attainment of the highest power conversion efficiency which stands at 10.71% [4]. The scattering and absorption efficiencies of solar cells can be also increased by the deposition of metallic nanoparticles such as gold, silver, aluminum, etc. Among these aluminum nanoparticles exhibits a superior ability to enhance surface plasmon resonance in addition to being cost efficient and abundant [5]. A substantial improvement in the light absorption capacity of perovskite solar cells has been achieved by geometrically optimizing the metal nanoparticles incorporated within the active perovskite layer which shows 38% energy conversion efficiency [6].

This paper aims to simulate a perovskite solar cell using $\text{CH}_3\text{NH}_3\text{PbI}_x\text{Br}_{1-x}$ as the absorber layer [7], ZnO_2 as the material for ETL and NiO_x as the material for HTL and an analysis is made in terms of some performance parameters such as varying temperature and varying thickness of absorber material.

Experimentation

Device structure

The structure of perovskite based solar cell is shown in figure 1 which consists of $\text{CH}_3\text{NH}_3\text{PbI}_x\text{Br}_{1-x}$ as absorber or perovskite material which is placed in between that of two layers called HTL and ETL with materials of NiO_x and ZnO_2 . The other layer is ITO. The left contact and right contact structure of the cell is shown in figure 2. After absorbing the light by the perovskite layer, the electron and hole pairs are produced in that absorber layer. These pairs of electrons and holes are retrieved from ETL as well as HTL layers and delivered to the suitable electrodes [8]. The parameter values of different materials are shown in figure 3.

Results and Discussion

The simulation of perovskite based solar cell is carried out in SCAPS version 3.3.07. The action panel of SCAPS 3.3.07 is shown in figure 4. There are some general steps for simulating the solar cell structure. In the first step we need to set the input parameter for the cell, then we have to set the working conditions, after that need to define the activity to be observed, then get the result and finally the analysis and comparison results [9]. The simulation includes different curve characteristics and performance parameter analysis.

Different curve characteristics

J-V curve

The simulation results of current density - voltage curve (J-V curve) at standard temperature of 300 K, zero voltage, $1.000\text{E}+6$ frequency and 5 number of points is shown in figure 5 with efficiency of 20.72, fill factor of 18.27.

C-F curve

The simulation results of C-F curve that includes capacitance - frequency, conductance - frequency, Nyquist plot and conductance/omega - frequency is shown in figure 6.

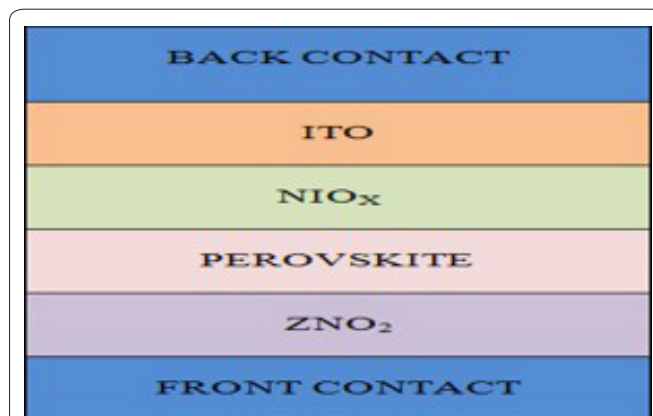


Figure 1: Structure of perovskite solar cell.

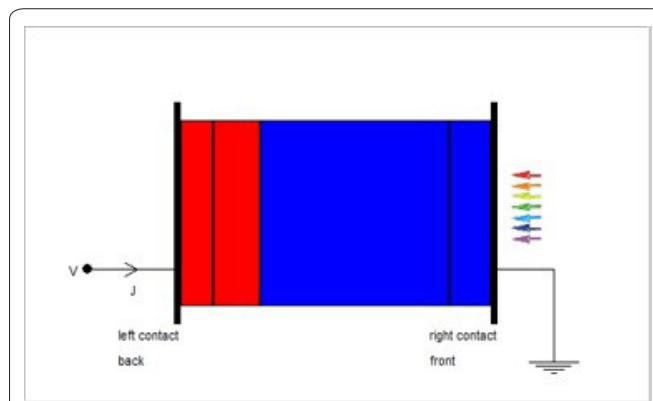


Figure 2: Structure of the cell.

PARAMETERS	MATERIALS			
	ITO	NiOx	Perovskite	ZnO2
Thickness	55 nm	80 nm	320 nm	70 nm
Bandgap	3.5 eV	3.5 eV	1.55 eV	3.2 eV
Electron Affinity	2.3eV	2.2 eV	3.9 eV	4.0 eV
Dielectric permittivity	9.0	9.0	6.5	8.5
N_c	$2.2\text{E}+18 \text{ cm}^{-3}$	$2.2\text{E}+18 \text{ cm}^{-3}$	$2.2\text{E}+18 \text{ cm}^{-3}$	$2.2\text{E}+18 \text{ cm}^{-3}$
N_v	$1.8\text{E}+19 \text{ cm}^{-3}$	$1.8\text{E}+19 \text{ cm}^{-3}$	$1.8\text{E}+19 \text{ cm}^{-3}$	$1.8\text{E}+19 \text{ cm}^{-3}$
Electron Thermal Velocity	$1\text{E}+7 \text{ cm/sec}$	$1\text{E}+7 \text{ cm/sec}$	$1\text{E}+7 \text{ cm/sec}$	$1\text{E}+7 \text{ cm/sec}$
Hole Thermal Velocity	$1\text{E}+7 \text{ cm/sec}$	$1\text{E}+7 \text{ cm/sec}$	$1\text{E}+7 \text{ cm/sec}$	$1\text{E}+7 \text{ cm/sec}$
Electron Mobility	$3\text{E}+1 \text{ cm}^2/\text{V-sec}$	$4.7\text{E}+0 \text{ cm}^2/\text{V-sec}$	$2\text{E}+0 \text{ cm}^2/\text{V-sec}$	$1\text{E}+2 \text{ cm}^2/\text{V-sec}$
Hole Mobility	$5\text{E}+0 \text{ cm}^2/\text{V-sec}$	$4.7\text{E}+0 \text{ cm}^2/\text{V-sec}$	$2\text{E}+0 \text{ cm}^2/\text{V-sec}$	$3\text{E}+1 \text{ cm}^2/\text{V-sec}$
Donor Density	0	0	$1\text{E}+15 \text{ cm}^{-3}$	$1\text{E}+16 \text{ cm}^{-3}$
Acceptor Density	$2.0\text{E}+16 \text{ cm}^{-3}$	$5.6\text{E}+16 \text{ cm}^{-3}$	0	0

Figure 3: Material parameters.

C-V curve

The simulation results of C-V curve that includes capacitance voltage, Mott-Schottky, conductance voltage and doping profile and depletion width is shown in figure 7.

Parameter analysis

The performance parameter analysis of this perovskite based solar cell includes the effect of temperature and effect of thickness in absorber layer.

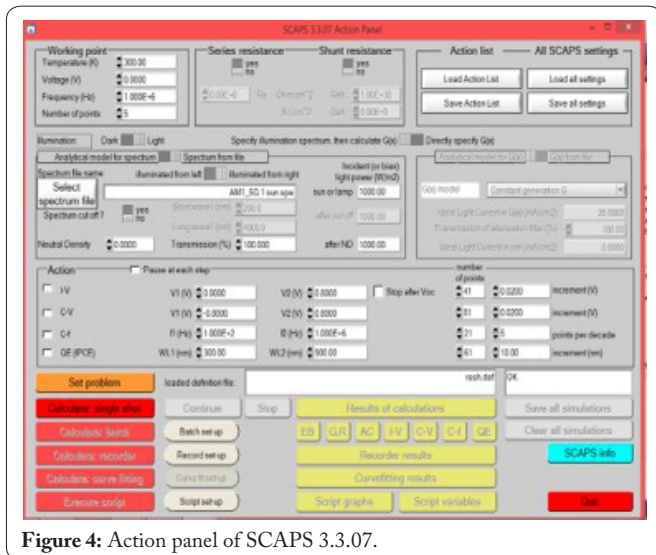


Figure 4: Action panel of SCAPS 3.3.07.

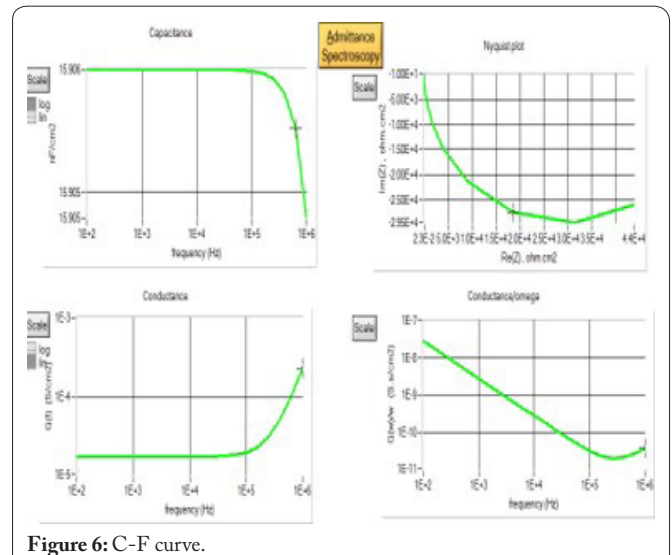


Figure 6: C-F curve.

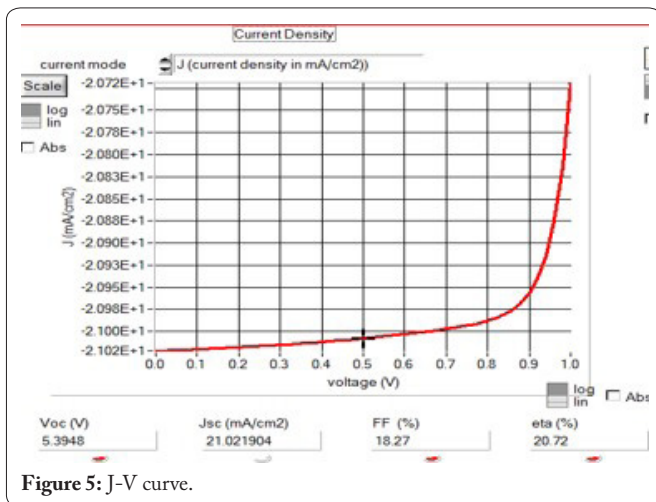


Figure 5: J-V curve.

Effect of temperature

In this paper, different temperature values like 300 K, 400 K and 500 K are taken and compared the solar cell with different parameters like efficiency in %, open circuit voltage in V, short circuit current in mA/cm², and fill factor in %.

The results show that the efficiency is 20.72% at 300 K, 17.39% at 400 K and 13.63% at 500 K. The fill factor parameter is 18.27% at 300 K, 74.47% at 400 K and 72.20% at 500 K. The short circuit current is 21.021904 mA/cm² at 300 K, 21.025927 mA/cm² at 400 K and 21.030017 mA/cm² at 500 K. The open circuit voltage is 5.3948 V at 300 K, 1.1104 V at 400 K and 0.8978 V at 500 K. The J-V curve at 300 K is shown in figure 5, at 400 K is shown in figure 8 and for 500 K it is shown in figure 9.

Effect of thickness

In this paper, various thickness for perovskite material for 300 nm, 400 nm and 500 nm are considered and compared the solar cell with different parameters mentioned above. The simulation result of perovskite solar cell at 320 nm thickness of absorber shows the efficiency of 20.72%, fill factor of 18.27%, short circuit current of 21.021904 mA/cm² and open circuit voltage of 5.3948 V is shown in figure 5.

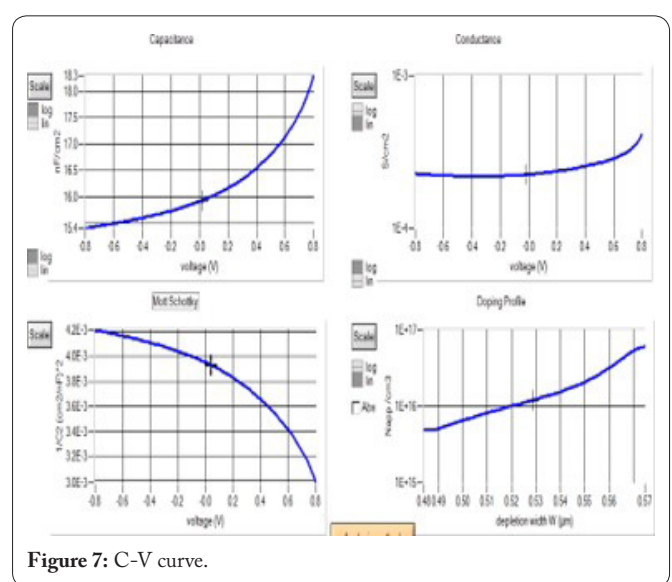


Figure 7: C-V curve.

The simulation result of perovskite solar cell at 400 nm thickness of absorber shows the efficiency of 22.09%, fill factor of 22.13%, short circuit current of 22.489118 mA/cm² and open circuit voltage of 4.4385 V is shown in figure 10.

The simulation result of perovskite solar cell at 500 nm thickness of absorber shows the efficiency of 23.16%, fill factor of 25.04%, short circuit current of 23.680481 mA/cm² and open circuit voltage of 3.9066 V is shown in figure 11.

Conclusion

In this proposed paper, the simulation of perovskite solar cell is done using the SCAPS software and analyzed the performance parameters such as effect of temperature and effect of thickness on absorber layer. The comparison of performance parameters is shown in figure 12. From that we can conclude that as temperature increases, the efficiency of this perovskite solar cell decreases. For the other parameter, increasing the thickness of absorber layer will increase the efficiency of this solar cell. The best result is obtained when varying the absorber thickness up to 500 nm which gives the efficiency of 23.16%.

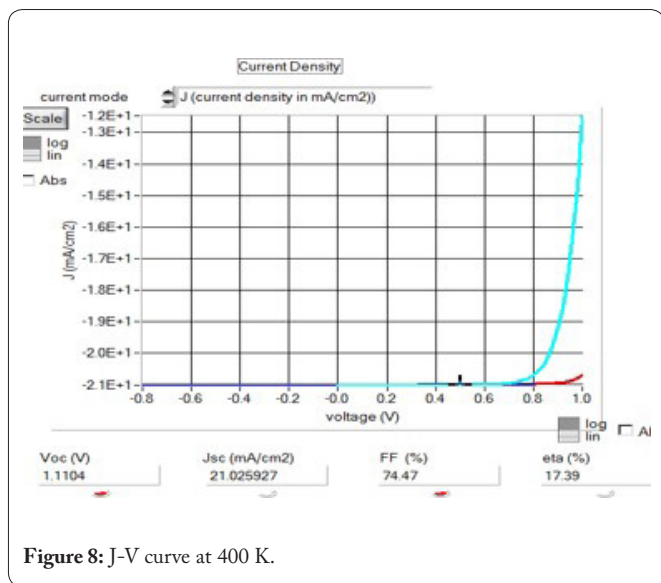


Figure 8: J-V curve at 400 K.

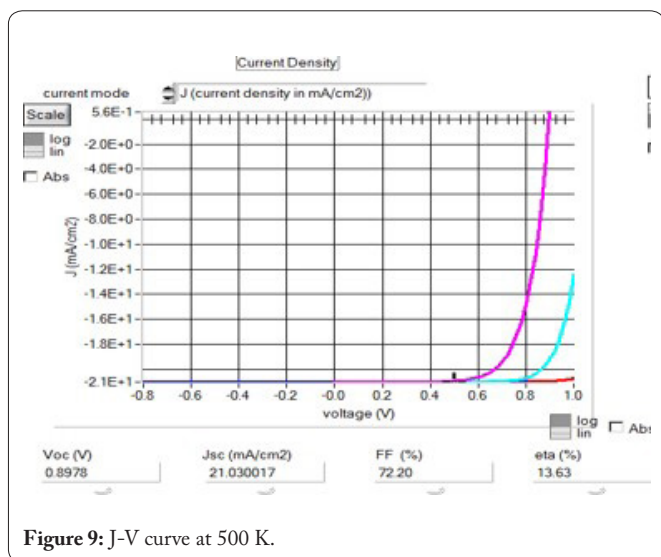


Figure 9: J-V curve at 500 K.

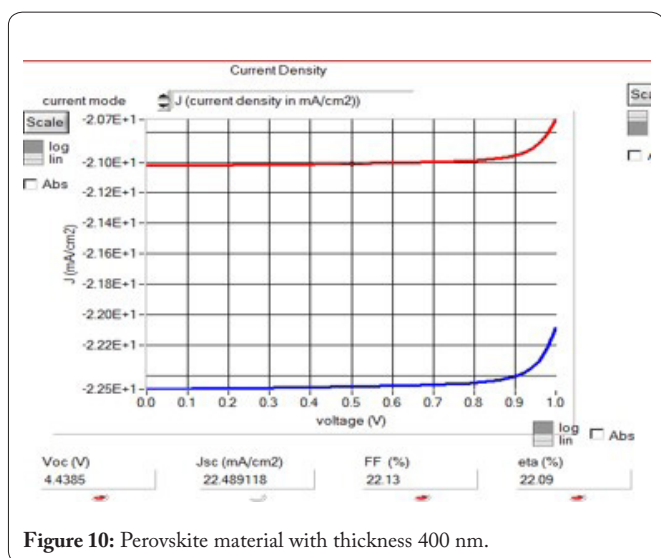


Figure 10: Perovskite material with thickness 400 nm.

Acknowledgements

None.

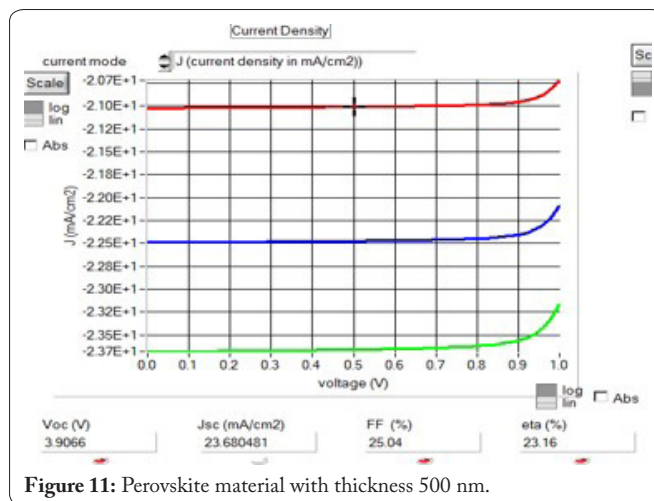


Figure 11: Perovskite material with thickness 500 nm.

Parameters	Effect of Temperature			Effect of Thickness on Absorber		
	300K	400K	500K	320nm	400nm	500nm
Efficiency (%)	20.72	17.39	13.63	20.72	22.09	23.16
Fill Factor (%)	18.27	74.47	72.20	18.27	22.13	25.04
Short Circuit Current (mA/cm ²)	21.021904	21.025927	21.030017	21.021904	22.489118	23.680481
Open Circuit Voltage (V)	5.3948	1.1104	0.8978	5.3948	4.4385	3.9066

Figure 12: Comparison of performance parameters.

Conflict of Interest

None.

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