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ENHANCED PERFORMANCE OF TIN HALIDE PEROVSKITE SOLAR CELL MODEL USING SCAPS-1D

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Abstract—*As of now exhibiting solar energy to the electrical energy conversion performance of more than 20%, perovskite based photovoltaic's are the emerging trend to produce clean and cheap energy. However the toxicity issue of most used lead perovskite material is the main challenge to use effectively as an absorber layer. A good alternative for the lead is tin, which is also a transition metal and having good semi conducting behavior. $CH_3NH_3SnI_3$ based perovskite solar cell is simulated using the software tool for the numerical simulation of thin film photovoltaic's Glass/ITO/TiO_2/ $CH_3NH_3SnI_3$/Spiro-OMETAD/Ag, architecture is optimized to achieve the high efficiency. The performance influencing parameters such as absorber thickness, defect concentrations and the operating temperature are optimized. The predicted photovoltaic parameters by the simulation process are Jsc is 25.41 mA/cm^2 , Voc is 1.29V, fill factor is 78.71% and efficiency is 25.75%.*

Keywords — Tin Halide Perovskite, absorber, optimized, defect, temperature.

I. INTRODUCTION

Industrialization and increasing population are the reasons for the growth of energy demand. The viable alternative for the fossil fuels is the solar energy. Almost the solar cell market is occupied by the silicon made solar cells. Installation and production cost of silicon, encouraging the scientific community to think over alternative materials. The dye sensitized and perovskite solar cells are identified alternative devices for silicon solar cells with rapid increase in efficiency. The compounds having the structure ABX_3, are known as perovskite. Among the perovskite materials $CH_3NH_3SnI_3$ have drawn much attention as it is the good substitute for silicon due to its abundance and easy processing techniques [1-5]. First, the application of perovskite material in photovoltaic's was developed by Miyasaka and team in 2009 and achieved efficiency is 3.8% [6]. Later, in 2011Park et al, with the perovskite absorber, achieved an efficiency of 6.5%. From past few years improved fabrication methods increasing the efficiency of perovskite solar cells as 10%,18% and 22% [7-8].

II. METHODOLOGY

Computer based software program developed based on the fundamental solar cell equations known as solar cell capacitance simulator (SCAPS) used in this work to develop the model of solar cell. It is programmed by the M. Burgelman et al at the University of Gent, Belgium. SCAPS suitable to design and analysis of thin film photovoltaic's [15-17].

The continuity equations of electrons and holes are:

$$\frac{dj_n}{dx} = G - R \qquad (1)$$

$$\frac{dj_p}{dx} = G - R \qquad (2)$$

The Poisson equation is: $\frac{d^2\emptyset(x)}{dx^2} = \frac{e}{\epsilon_0\epsilon_r}(\rho(x) - n(x) + N_D - N_A + \rho_p - \rho_n \qquad (3)$

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$$J_n = D_n \frac{dn}{dx} + \mu_n n \frac{d\emptyset}{dx}$$

$$J_p = D_p \frac{dn}{dx} + \mu_p p \frac{d\emptyset}{dx}$$

III. ARCHITECTURE OF PEROVSKITE SOLAR CELL

To model this architecture, the tin based perovskite material $CH_3NH_3SnI_3$ is sandwiched between the n-type electron transport material i.e. TiO_2 and P-type hole transport material i.e. Spiro-OMETAD. The total architecture of the model is Glass/ITO/TiO_2/ $CH_3NH_3SnI_3$/Spiro-OMETAD/Ag.

Figure: 1 Schematic representation of Glass/ITO/TiO_2/ $CH_3NH_3SnI_3$/Spiro-OMETAD/Ag

taken from the previous experimental and theoretical work from literature [18-22].

IV. RESULTS AND DISCUSSIONS

Influence on PV parameters by modification of thickness of the absorber layer:

Absorber thickness is the main parameter which decides the efficiency of the device. Moderate thickness equal **.**

Simulation parameters:

To develop the tin based perovskite solar cell, using the simulation software SCAPS we need to give to the diffusion length of charge carriers is necessary to record best results. Opto-electronic properties also changes with the thickness of absorber layer. In this simulation model, the defect free absorber layer thick ness is in the range of 0.1 µm to 0.8 µm under one sun illumination. As we observe from the graphs the short circuit density increases slowly as the thickness increases representing the increased number of photons and improved generation process. The power conversion efficiency of the model increases from 0.1 µm to 0.3 µm and reaches to the efficiency 29.66%. Later due to the increased recombination

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efficiency decreases slowly. The remaining two parameters open circuit voltage and fill factor decreases with the thickness.

Table-1: Simulation parameters of a tin based perovskite solar cell.

Parameter	**Spiro-OMETAD**	**$CH_3NH_3SnI_3$**	**TiO_2**	**ITO**
Thickness (µm)	0.030	0.300	0.070	0.170
Band gap(eV)	3.0	1.230	3.260	3.650
Electron affinity(eV)	2.200	4.5	4.500	4.8
Dielectric Permittivity	3.0	10	9.0	8.9
CB effective density of states ($1/cm^3$)	2.200E+17	1.000E+14	2.200E+19	4.900e+19
VB effective density of states ($1/cm^3$)	1.800E+16	1.000E+17	1.800E+17	1.00E+19
Electron thermal velocity(cm/S)	2.00E+7	1.00E+7	1.00E+7	2.00E+7
Holethermalvelocity(cm/S)	1.00E+7	1.00E+7	1.00E+7	1.00E+7
Electron mobility(cm^2/VS)	1.00E-4	1.60E-+0	1.00E+2	1.00E+2
Hole mobility(cm^2/VS)	4.000E-4	1.600E+0	2.500E+1	2.500E+1
Shallow uniform donor density ND ($1/cm^3$)	0	0	2.00E+21	1.00E+18
Shallow uniform acceptor density NA($1/cm^3$)	3.00E+19	1.000E+18	0	0

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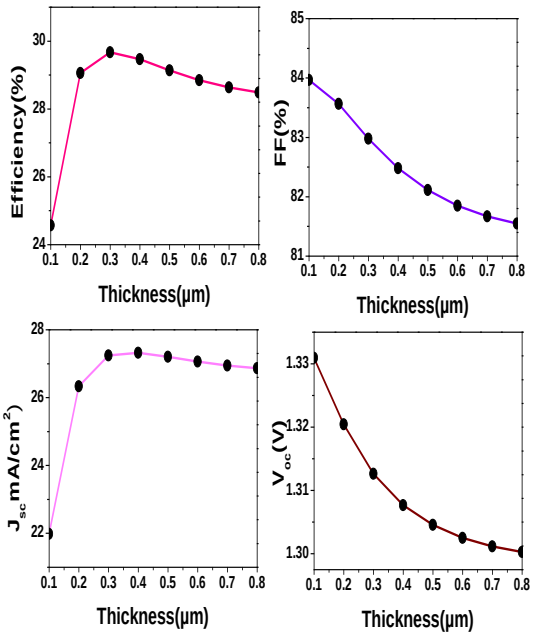

Figure: 2 Graph of change in performance parameters with the thickness of absorber layer

The fill factor is the representation of the quality of the device, as the thickness increases the increased surface recombination is the main reason to decrease the fill factor. The reason behind the reduction in the open circuit voltage is the increased resistances in the model. However, the power conversion efficiency is maximum when the thickness is 0.3μm. So, the optimal thickness for the architecture is 0.3 μm. At 0.5 μm the attained PV parameters are short circuit current density (J_{sc}) is 27.23 mA/cm^2, open circuit voltage (V_{oc}) is 1.31V,fill factor(FF) 82.97%, power conversion efficiency is 29.66%.

Influence on PV parameters by modification of defect density of the absorber layer:

Performance of a photovoltaic is heavily influenced by the defects such as grain boundaries, point/intrinsic (or) crystalline structure and the doping concentration of absorbing layer. From the literature, the quality and absorber (perovskite) layer is an important in finding the perovskite solar cell efficiency [23-24]. Frenkel defects present in the absorber layer are the reason for the loss in performance of photovoltaic's [25]. The defect density of a material is influenced by the chemical potential and the formation of energy. Long electron-hole diffusion length in the absorber is due to the formation of fewer defects i.e. at shallow level. These type of defects forms the high 'V_{oc}'. Baumann et al and agiorgousis et al described the deep level defects in the perovskite solar cell using the first principle study [26-27].

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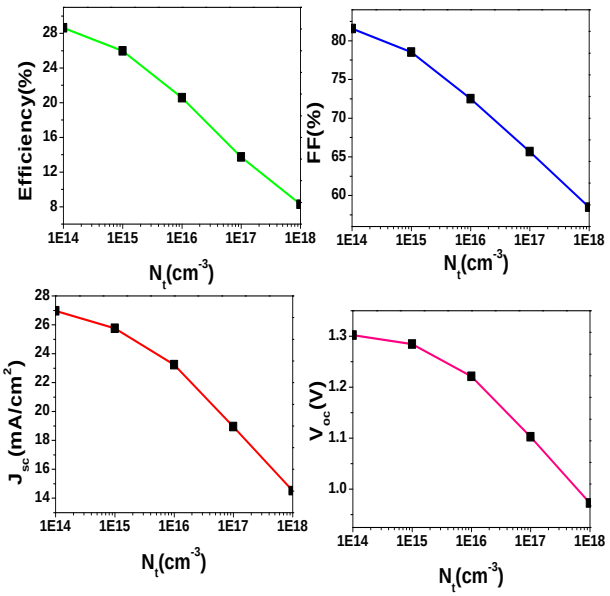

Figure: 3 Graph of change in performance parameters with the defect density of absorber layer

The larger defect density leads to the poor film quality and the increased charge recombination behaviour reduces the V_{oc}. Influence of defect density of the absorber layer can be studied by the Shockely-Read Hall recombination model [28-29].

The SRH recombination model is as follows:

$$R = \frac{np - n_i^2}{\tau_p(n + N_C e^{\frac{E_g - E_t}{KT}}) + \tau_n(P + N_v e^{\frac{E_t}{KT}})}$$

Here, n and p are the electron and hole densities

If qv>3KT, we can neglect n_i^2

E_t' is the energy level concentration

τ_n and τ_p are the life time of electron and hole.

In this simulation work, the defect density of absorber layer is varied from 10^{14} cm^{-3} to the 10^{18} cm^{-3} to observe changes in the PV parameters. As the defect concentration increases, the recombination's increases with this the performance of the device. When the defect density is set at 10^{14} cm^{-3} the PV parameters are J_{sc} is 26.96 mA/cm^2 , V_{oc} is 1.30V, fill factor is 81.55% and efficiency is 28.63%, when the defect density increases to the 10^{18} cm^{-3} then the attained PV parameters are J_{sc} is 14.51 mA/cm^2, V_{oc} is 0.97, fill factor is 58.46% and efficiency is 8.25%, the great loss in the performance of the device is due to the destroy of holes and electrons in the defects. So the optimum defect density of the perovskite absorber layer is set to be 10^{15} cm^{-3}. At this optimum defect density the achieved PV parameters are J_{sc} is 25.74 mA/cm^2, V_{oc} is 1.28V, fill factor is 78.52% and efficiency is 25.96%.

Variation of PV parameters with the operating temperature:

Generally, in simulation works 300K is selected as the operating temperature. But practically

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operating temperature is not fixed it depends on place, latitude, day, year. So, the changes in PV parameters with the temperature need to study. In this simulation work, we vary the temperature from 300K to 450K.

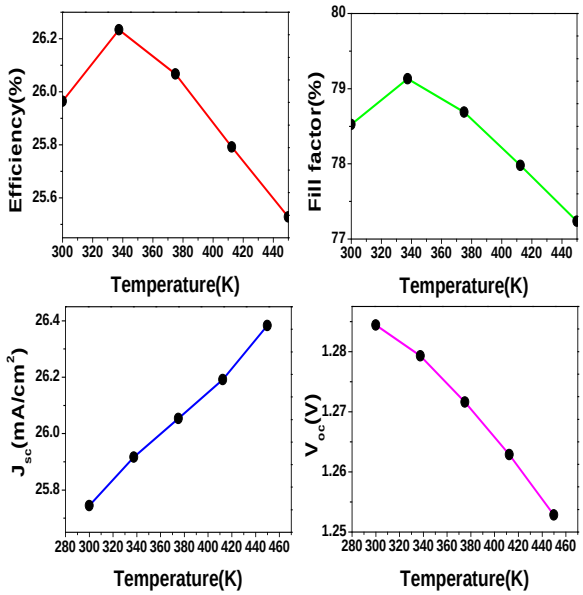

Figure: 4 Graph of change in performance parameters with the operating temperature

It was observed that at lower temperatures the model is showing the highest performance. This is because the increased temperature changes the mobility, band gap, band gap, carrier concentration. Due to the increased thermal generation of charges and reduced band gap is the main reason to increase the short circuit current density. Disturbances in the alignment of energy levels, improves the recombination and reduces the fill factor, V_{oc}, efficiency. In this case absorber layer is considered having the 10^{15} cm^{-3} defect density, which is optimized in the previous case. Finally, the optimum operation temperature of the model is set at 300K. The attained maximum parameters of the simulation model is J_{sc} is 25.74 mA/cm^2 , V_{oc} is 1.3V, fill factor is 78.52% and efficiency is 25.96%,

V. FINAL SIMULATED I-V CURVE

The perovskite solar cell model is simulated with the thickness of absorber layer as 0.3 µm, the defect density (cm^{-3}) of perovskite absorber layer is 10^{15} cm^{-3} and the operating temperature is 300K. The achieved results are J_{sc} is 25.41 mA/cm^2 , V_{oc} is 1.29V, fill factor is 78.71% and efficiency is 25.75%,

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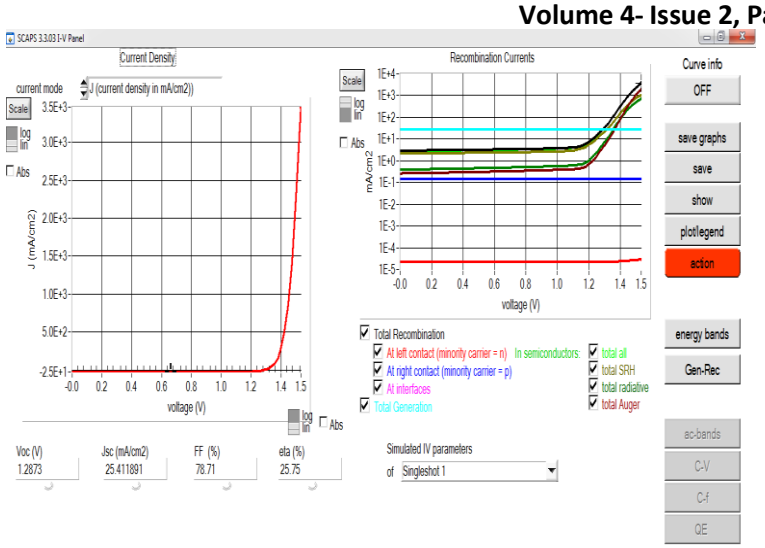

Figure:5 J-V curve

VI. CONCLUSION

Lead free perovskite solar cells having the architecture Glass/ITO/TiO_2/ $CH_3NH_3SnI_3$/Spiro-OMETAD/Ag are analyzed using the SCAPS. The outcome of solar cell simulation is showing that the moderate thickness of perovskite solar cell improves the performance, because of less recombination and effective diffusion length of charge carriers. But too much thickness of absorber layer is showing the adverse effect on the efficiency of the device. The optimum thickness of the absorber layer is 0.3 µm. The defect density of a solar cell is also important to achieve the high efficiency. By improving the quality of the film of the absorber layer with the low defects can able to get the high efficiency. In this model the optimum defect density is considered as $10^{15}cm^{-3}$. Similarly, the operating temperature of the model is set as 300K. With all the above optimized parameters, a good encouraging result of efficiency is achieved nearly equal to the 26%. This simulation work will give information in optimizing parameters, while fabricating the tin based perovskite solar cell.

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