THICKNESS OPTIMIZATION OF PEROVSKITE SOLAR CELLS USING GPVDM SIMULATION

Yogesh Patel*[1], Sachin Desai[2], Dr. Uday Trivedi[3]

[1]Department of Balbhavan, Children's Research University, Gandhinagar – 382021*
[2]Department of Balbhavan, Children's Research University, Gandhinagar – 382021
[3]Goverment Polytechnic, Ahmedabad

Corresponding Author:

Abstract

Due to their great potential efficiency and low cost of production, perovskite solar cells have become an attractive technology for next-generation photovoltaics. In this study, we use the modelling tool GPVDM (Generalised Photovoltaic Device Model) to look at how thickness variations affect the performance of perovskite solar cells. By systematically varying the thickness of the perovskite layer and other functional layers, we aim to optimize the device performance. The simulation focuses on key parameters such as absorption efficiency, charge transport characteristics, carrier recombination rates, photocurrent generation, and open-circuit voltage. The perovskite (PVK) absorber layer is composed of CH3NH3PbI3, the hole transport layer is composed of spiro-OMeTAD, and the electron transport layer is composed of TiO2. These layers are sandwiched together to form the simulated solar cell. Solar cells' conversion efficiency can be increased by adjusting the layer thicknesses of various materials. The outcomes show that it is feasible to have layer thicknesses with a maximum power conversion efficiency of 23.32%.

Introduction:

Due to their exceptional power conversion efficiency and potential for low-cost manufacturing, perovskite solar cells have become a very promising technology in the field of photovoltaics. These solar cells are based on thin films of hybrid organic-inorganic perovskite materials, which exhibit excellent light-absorbing and charge transport propertiesin photovoltaic devices like solar cells, LEDs, supercapacitors, and FETs, perovskite material is employed quite well. One of the best energy harvesting technologies for the foreseeable future is the perovskite solar cell. Perovskite solar cells are greater than 25% efficient[1–2].
In recent years, simulation tools such as GPVDM (Generalized Photovoltaic Device Model) have become invaluable in investigating the behavior and performance of perovskite solar cells. GPVDM provides a comprehensive platform to model and simulate the electrical and optical characteristics of photovoltaic devices, including perovskite solar cells. By utilizing GPVDM simulations, researchers can explore the effects of different parameters, including layer thickness, on the performance of perovskite solar cells in a controlled and efficient manner.
In this research paper, we aim to investigate the influence of thickness variations on the performance of perovskite solar cells using GPVDM simulations. Our study focuses on optimizing the device parameters by systematically varying the thickness of the perovskite layer and other functional layers. We analyze key performance metrics such as absorption efficiency, charge transport characteristics (electron and hole mobilities), carrier recombination rates, photocurrent generation, and open-circuit voltage.
Device structure
For the GPVDM simulation, which aids in the optimization of the electrical and optical properties, we employ the materials ITO/TiO2/perovskite/Spiro-MeOTAD/Al [3].
Device Simulation Technique
In our material layer models, we emphasise the use of defect-free material layers. TiO2 functions as the electron transporting material (ETM), Spiro-MeOTAD functions as the hole transporting material (HTM), and perovskite functions as the active photovoltaic layer that generates charge carriers (electron and hole). In addition to conducting electricity and being economically feasible for device manufacturing, these materials are also environmentally beneficial [4].
We are utilising the electrical simulation application GPVDM to examine the combined effect of the device modelling and to explain the PCE (power conversion efficiency) and stability of the device. The increase in power conversion efficiency that was made possible by changing the layer thickness of peroskite materials CH3NH3PbI3-based solar cell. The initial layer thickness at $1x10^{-7}$ m is shown in Table 1, and the simulation results are shown in Table 4. The PCE value in Table 4 is 14.16%.

Table 1. Layer thickness of the typical perovskite solar cell.

Layer Name Layer	**Thickness(m)**	**Optical Material**	**Type**
ITO	1e-8	Oxides/ITO/ito	Contact
TiO_2	2e-7	Oxides/tiox	Active
Perovskite	1e-07	Perovskites/CH3NH3PbI3/Ball	Active
Spiro-MeOTAD	2e-07	Small molecules/spiromeotad	Active

Al	1e-07	Metal/Al/std	Other

For the simulation of photovoltaic materials like CH3NH3PbI3 perovskite used in solar cells, LEDs, photodiodes, and other energy harvesting devices, we use GPVDM software. The GPVDM simulation programme has successfully solved the Poisson equation (1), the bipolar drift-diffusion equations(2,3),and the carrier continuity equations(4,5).

$$\frac{d}{dx}\varepsilon_0\varepsilon_r\frac{\partial\varphi}{\partial x} = q(n-p) \quad (1)$$

$$J_n = q\mu_c n\frac{\partial E_c}{\partial x} + qD_n\frac{\partial n}{\partial x} \quad (2)$$

$$J_p = q\mu_n p\frac{\partial E_v}{\partial x} - qD_p\frac{\partial p}{\partial x} \quad (3)$$

$$\frac{\partial J_n}{\partial x} = q\left(R_n - G + \frac{\partial n}{\partial x}\right) \quad (4)$$

$$\frac{\partial J_p}{\partial x} = -q\left(R_p - G + \frac{\partial p}{\partial x}\right) \quad (5)$$

The preceding equations thorough explanation serves as a model for common perovskite solar cells (PSCs) [4-5].
The computational structure of the device's planar structure is shown in Fig. 1 as ITO/ETM/ CH3NH3PbI3/ HTM/Aluminum, where TiO2 serves as the electron transporting (ETM)layer and Spiro-MeOTAD serves as the hole transporting material (HTM) respectively.

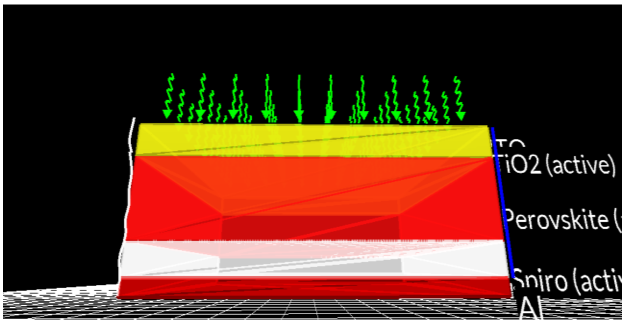

Fig. 1. Planar structure of perovskite Solar cell

The GPDVM software window, which is depicted in Fig. 1, can be used to select the initial layer thickness of the nanostructured device. Tables 2 and 3 provide an explanation of the initial simulation parameters. By using the GPVDM software database, we may select the electrical and optical parameters. Our research is based on Table 4's depiction of the nanostructured device's (PSCs) changing in perovskite materials layer thickness. Therefore, we discovered that the device's electrical characteristics changed as the layer thickness was adjusted. The greatest efficiency was determined to be 23.32% at a perovskite thickness of $5\text{x}10^{-7}$ m.

Table 2: Simulation Parameters for GPVDM Software

Parameters	Electrical Value
Electron trap density	1×10^{20} $m^{-3}eV^{-1}$
Hole trap density	1×10^{20} $m^{-3}eV^{-1}$
Electron tail slope	0.06 eV
Hole tail slope	0.06 eV
Electron mobility	0.0002 $m^2V^{-1}s^{-1}$
Hole mobility	0.0002 $m^2V^{-1}s^{-1}$
Number of traps	5
Free electron to Trapped electron	1×10^{-20} m^{-2}
Trapped electron to Free hole	1×10^{-22} m^{-2}
Trapped hole to Free electron	1×10^{-22} m^{-2}
Free hole to Trapped hole	1×10^{-20} m^{-2}
Effective density of free electron states	1×10^{20} m^{-3}
Effective density of free hole states	1×10^{-22} m^{-3}

Table 3: Electric Parameter for Simulation GPVDM Software

Fill Factor	6.384×10^{-2}	a.u.
Power conversion efficiency	23.32	%
Max Power	2.332×10^{2}	Wm^{-2}
V_{OC}	1.645×10^{1}	V

J_{OC}	-2.221×10^{2}	Am^{-2}
Recombination time constant at V_{OC}	-1.0	S
Recombination rate at V_{OC}	-1.0	S
Average carrier density at Pmax	1.279×10^{-3}	$M^2V^{-1}s^{-1}$
Trapped electron at Voc	-1.0	m^{-3}
Trapped hole at Voc	-1.0	m^{-3}
Free electrons at Voc	-1.0	m^{-3}
Free holes at Voc	-1.0	m^{-3}
Total carriers (n + p)/2 at Voc	-1.0	m^{-3}

Table 4: The Electric Parameters with Thickness Changes in Pervoskite Layer for Pervoskite Solar Cell

Thickness (m)	V_{OC} (Volt)	I_{SC} (Ampere)	V_{MPP} (Volt)	I_{MPP} (Ampere)	F.F. (a.u.)	Max $Power_{MPP}$ (Watt-m^{-2})	Conversion Efficiency %
1×10^{-7}	4.533×10^{1}	-1.335×10^{2}	1.064	-1.331×10^{2}	2.340×10^{-2}	1.416×10^{2}	14.16
2×10^{-7}	1.730×10^{1}	-1.344×10^{2}	1.064	-1.338×10^{2}	6.122×10^{-2}	1.424×10^{2}	14.24
3×10^{-7}	1.038×10^{1}	-1.481×10^{2}	1.062	-1.471×10^{2}	1.016×10^{-1}	1.563×10^{2}	15.63
4×10^{-7}	9.466	-1.736×10^{2}	1.059	-1.724×10^{2}	1.111×10^{-1}	1.827×10^{2}	18.27
5×10^{-7}	1.645×10^{1}	-2.221×10^{2}	1.054	-2.213×10^{2}	6.384×10^{-2}	2.332×10^{2}	23.32
6×10^{-7}	1.339×10^{1}	-1.724×10^{2}	1.059	-1.716×10^{2}	7.877×10^{-2}	1.819×10^{2}	18.19
7×10^{-7}	1.223×10^{1}	-1.440×10^{2}	1.063	-1.433×10^{2}	8.650×10^{-2}	1.523×10^{2}	15.23
8×10^{-7}	2.469	-2.284×10^{2}	1.054	-2.167×10^{2}	4.052×10^{-1}	2.285×10^{2}	22.85
9×10^{-7}	2.465	-1.819×10^{2}	1.059	-1.726×10^{2}	4.079×10^{-1}	1.830×10^{2}	18.30

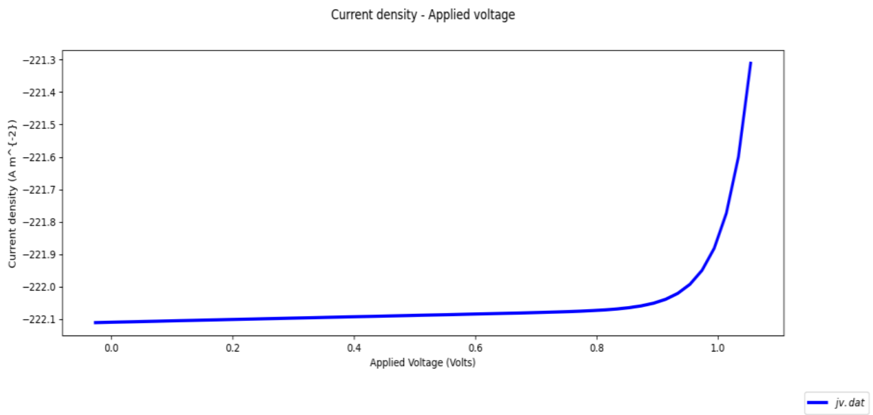

Figure 2: J-V Charctaristics for perovskite solar cell

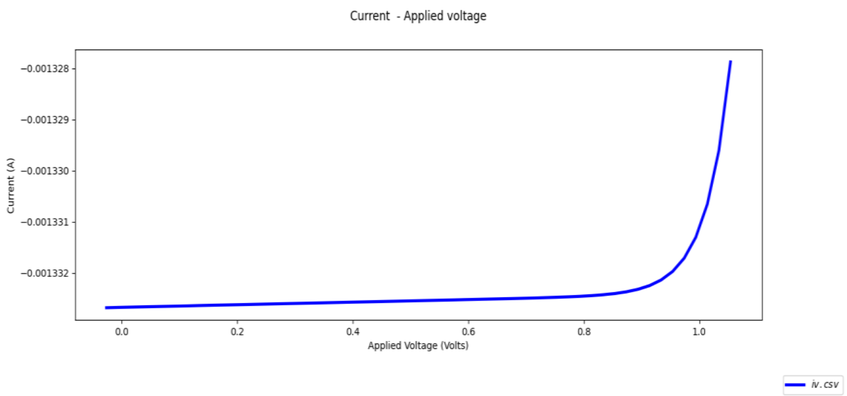

Figure 3: I-V Charctaristics for perovskite solar cell

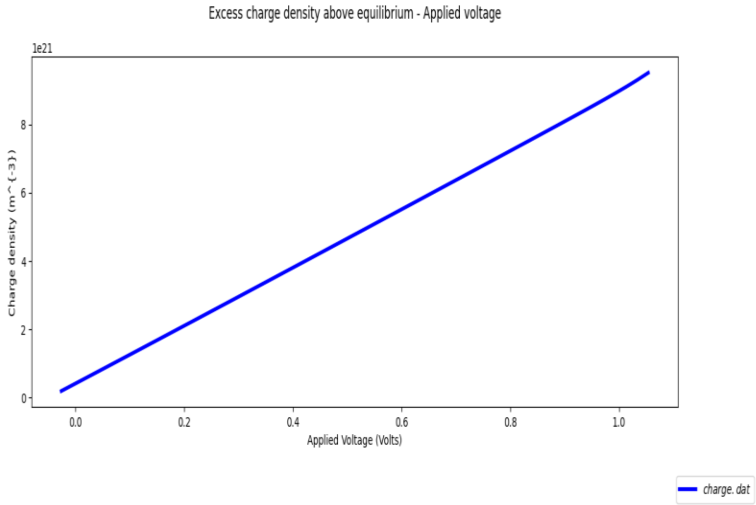

Figure 4: Excess Charge Density above equaillibrium

Conclusion :

We discovered that adjusting the active layer thickness from 1x10-7 m to 9x10-7 m alters the device's performance; we observed that the maximum efficiency was attained at 5x10-7 m, or 23.32% at 300 K, indicating that perovskite may function as an energy-harvesting device material. Additionally, we may improve the device's effectiveness by adjusting the thickness of Persoskite layer, By identifying the thickness that yields the highest efficiency, our research contributes to the ongoing efforts to improve the design and fabrication of perovskite solar cells. These findings provide valuable insights for researchers and engineers working on the development of high-efficiency photovoltaic devices.

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