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GPVDM simulation of layer thickness effect on power conversion efficiency of $CH_3NH_3PbI_3$ based planar heterojunction solar cell

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Abstract – *Perovskite-based solar cell technologies have been a very attractive area of research in recent years. Organic-inorganic perovskite materials are in an increased evolution in power conversion efficiency. Inorganic materials have been tested at the laboratory level but their power conversion efficiency is still limited. In this paper, we used the GPVDM software to study the effect of some parameters on power conversion efficiency in a planar heterojunction solar cell based on $CH_3NH_3PbI_3$ as an absorbing layer. The modifications were made by considering layers of perovskite without defects. The results show that the efficiency of the power conversion can be improved by adjusting layer thickness; in our case power conversion efficiency was increased from 9.96 % to 12.9 %.*

Keywords: *Perovskite, MAPbI3, PCE, GPVDM Software, layer thickness*
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I. Introduction

The very peculiar structure of perovskites is at the origin of many researches in various fields of physics and their applications. It was discovered in 1940 that synthetic ceramics of perovskite structure such as barium titanate (BaTiO3) had remarkable piezoelectric properties, that is to say that they were electrically polarized easily under the action of mechanical stresses. . Perovskite-type single crystals have been more recently manufactured with even more interesting piezoelectric properties.

The research in laboratories on hybrid organic-inorganic perovskites has become very intensive. This new technology of perovskite solar cells has seen a rapid progression and each time new percentage of power conversion efficiency that appear. To see the surprising progression of this area reminds that in 2009 a study was made on a cell based on CH3NH3PbBr3 with a high photovoltage of 0.96 V and the value of the efficiency was 3.8% [1] . After two years in 2011, a Perovskite cell of size 2-3 nm ($CH3NH3PbI_3$) nanocrystal gave a solar-electric conversion efficiency of 6.54% [2]. During the year 2013, energy conversion efficiencies reached an astounding 16.2% [3]. In the same year, an optimization of the TiO_2 layer treatment conditions, yields a PCE of 19.3% [4, 6]. Almost five years of research, it became between 22.1 and 22.6 % [7]

Different parameters can increase PCE in perovskite based solar cells; one of them is layer thickness of different layers. In the present paper we used GPVDM which is a powerful software simulation for photovoltaics, where we investigated effect of different layer thickness on power conversion efficiency of a planar heterojunction solar cell using $CH_3NH_3PbI_3$ as absorber layer.

II. Device simulation parameters

General-Purpose Photovoltaic Device Model (GPVDM) is free general purpose software for solar cell simulation based on solving Poisson equation (1) and the bipolar drift diffusion equations (2,3) and the carrier continuity equations (4,5) in 1D and time domain.

$$\frac{d}{dx}.\varepsilon_0\varepsilon_r.\frac{d\phi}{dx}=q(n-p) \quad (1)$$

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

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

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

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

More detail on above equation resolving and device modeling can be found in more detail in [8-11].

GPVDM software graphical interface is shown in Figure 1.

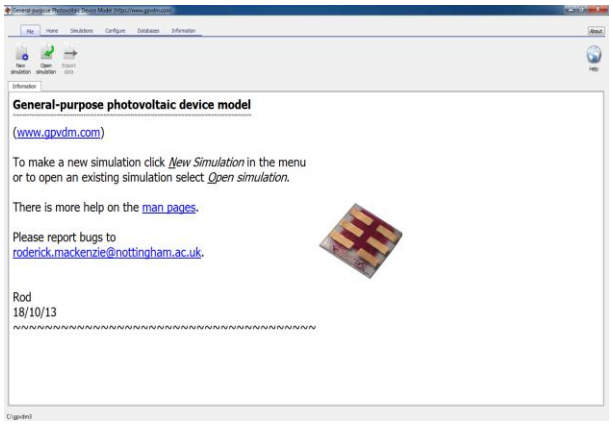

Figure 1. GPVDM Home window.

In Figure 2 is shown the planar heterojunction architecture of a $CH_3NH_3PbI_3$ based solar sell. The layer configuration adopted in this simulation is Glass/TCO/ETM/$CH_3NH_3PbI_3$/HTM/Silver where ETM layer is the TiO_2 and the HTM layer is the spiro-OMeTAD. In Table 1 is shown initial parameters that were carefully picked from practical and theoretical references [12-21]. Perovskite electrical and optical parameters are set from [16] and from GPVDM software database based on [22]. Glass layer and silver layer thickness are taken 6×10^{-8} m and 2×10^{-7} m respectively.

Our simulation is based on study of effects of different layer thickness on power conversion efficiency. Initial layer thickness given in Table 1 yields the J-V characteristic curve shown in Figure 3, in which power conversion efficiency PCE is 9.96 %, fill factor is 75.86 %, Open-circuit voltage V_{oc} is 0.47 V and short-circuit density of current is -277 A/m^2.

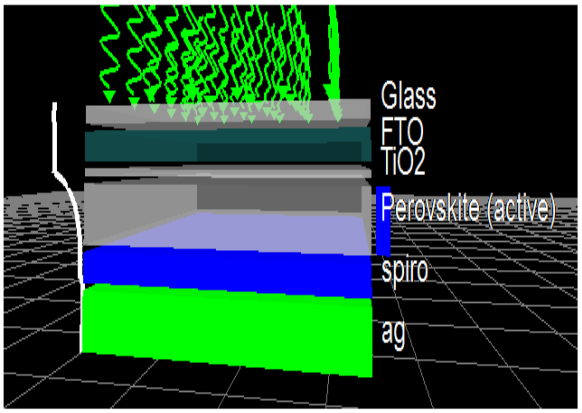

Figure 2. Planar heterojunction architecture of the studied solar cell

Table 1. Simulation parameters

Parameters	FTO	TiO_2	$CH_3NH_3PbI_3$	spiro-OMeTAD
Layer thickness (m)	1e-7 *(variable)*	2.5e-8*(variable)*	1e-7*(variable)*	1e-7*(variable)*
Relative permittivity ε_r	3	9	3	3
Band gap energy (eV)	0	3.2	2.1	3.17
Electron affinity (eV)	4.7	4.26	3.7	2.05
Electron mobility (m^2/V.s)	6.86e-07	20e-4	6.86e-07	2e-08
Hole mobility (m^2/V.s)	3.75e-02	10e-4	3.75e-02	2e-08
Donor concentration (m^{-3})	5e26	1e22	5e26	0
Acceptor concentration (m^{-3})	5e26	0	5e26	2e25

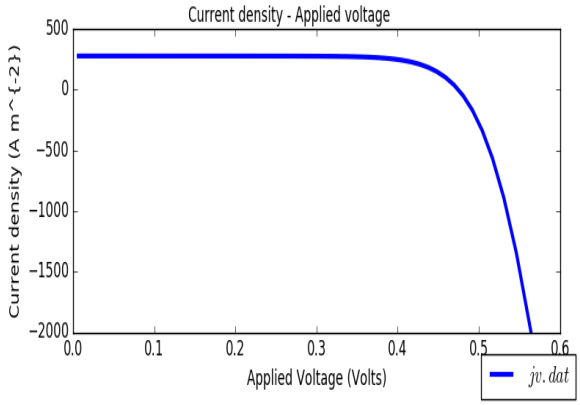

Figure 3. J-V characteristics for initial layer values

III. Results and discussion

Optimization method used in our simulation is to fix all parameters and modify one by one until we have the parameters that gives maximal PCE. In Figure 4 is presented the curve of effect of perovskite layer thickness on PCE.

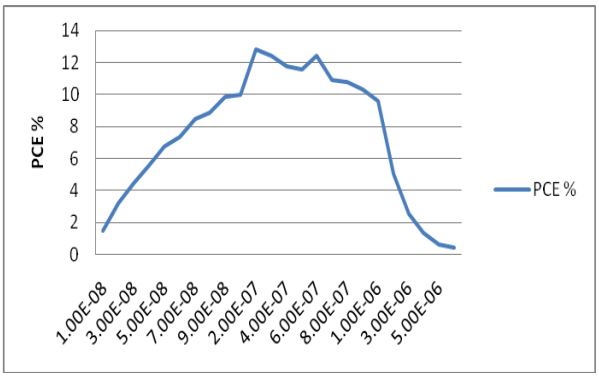

Figure 4. Effect of $CH_3NH_3PbI_3$ layer thickness on PCE

From Figure 4 we can note that a perovskite layer thickness of 2×10^{-7} m gives the maximal value of PCE which is 12.83 %, with a fill factor of 74.79 %, an open-circuit voltage of 0.47 V and a short-circuit density of current of -370 A/m^2.

We fix the $CH_3NH_3PbI_3$ layer thickness on 2×10^{-7} m and we change the FTO layer thickness to obtain curve in Figure 5.

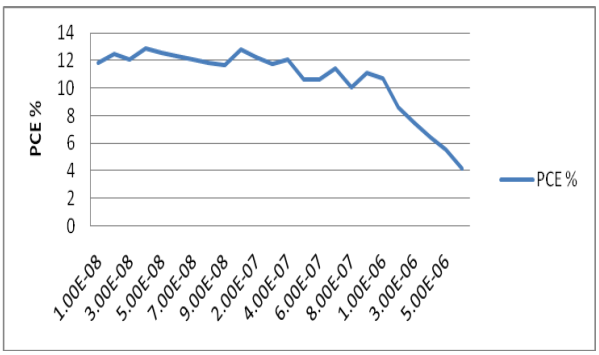

Figure 5. Effect of FTO layer thickness on PCE

From Figure 5 we obtained a maximal value of PCE which is 12.90 % corresponding on FTO layer thickness of 4×10^{-8} m, with a fill factor of 74.79 %, an open-circuit voltage of 0.47 V and a short-circuit density of current of -372 A/m^2.

By setting FTO layer thickness to 4×10^{-8} m and changing the spiro-OMeTAD layer thickness we obtained curve in Figure 6.

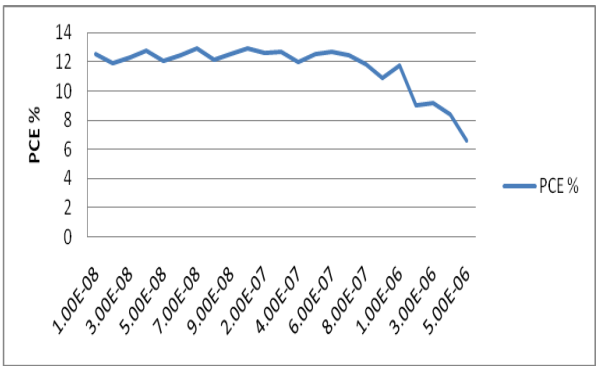

Figure 6. Effect of spiro-OMeTAD layer thickness on PCE

In Figure 6 we can note that the maximal PCE is 12.90 % in the spiro-OMeTAD layer thickness of 10^{-7} m with a fill factor of 74.79 %, an open-circuit voltage of 0.47 V and a short-circuit density of current of -372 A/m^2

When spiro-OMeTAD layer thickness is set to 10^{-7} m and changing of TiO_2 layer thickness we obtained curve in Figure 7.

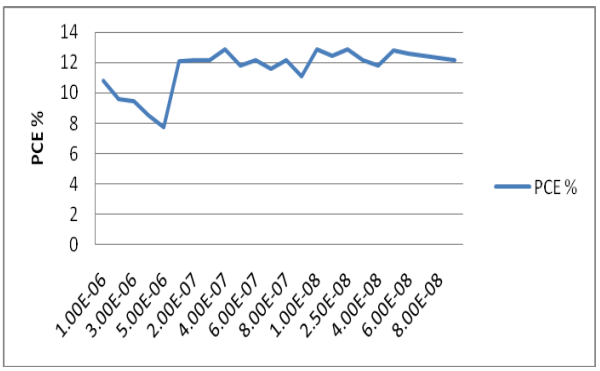

Figure 7. Effect of TiO_2 layer thickness on PCE

Curve of Figure 7 shows that Maximal PCE of 12.9 % is obtained in TiO_2 layer thickness of 2.5×10^{-8} m, where fill factor is 74.79 %, open-circuit voltage is 0.47 V and short-circuit density of current is -372 A/m^2.

In Figure 4 to Figure 7 is presented different layer thickness effect on PCE for a $CH_3NH_3PbI_3$ based planar heterojunction solar cell where we saw that efficiency increased from 9.96 % in initial parameters to 12.9 % with optimized parameters.

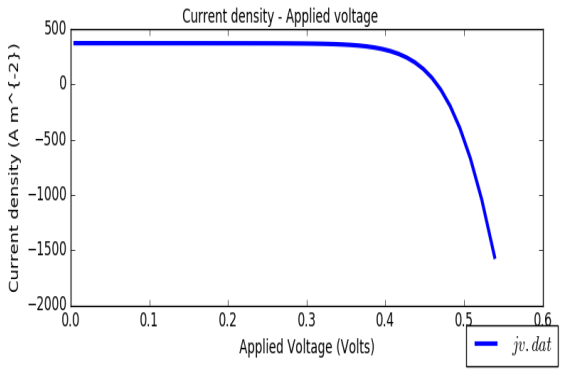

Figure 8. J-V characteristics for optimized layer values

In Figure 8 above we can see J-V characteristic of the studied solar cell with optimized parameters.

IV. Conclusion

Perovskite power conversion efficiency was analyzed using the GPVDM solar cell software simulation. Results indicate that a good choice of layer thickness of different materials used in the solar cell increases considerably the PCE ratio. From Simulation results is found that an improvement of 2.94 % is made by setting layer thickness of FTO to 4×10^{-8} m, of TiO_2 to 2.5×10^{-8} m, of Perovskite to 2×10^{-7} m and of spiro-OMeTAD to 10^{-7} m. Further PCE enhancements can be done by changing layer structure and materials.

V. Nomenclature

ε_0 is the permittivity of free space
ε_r is the relative permittivity
ϕ is the voltage profile
q is the elementary charge on an electron
n is the free electron concentration
p is the free hole concentration
J_n is the electron current flux density
J_p is the hole flux density
μ_c is the electron mobility
μ_h is the hole mobility
E_c is the free electron mobility edge
E_v is the free hole mobility edge
D_n is the electron diffusion coefficient
D_p is the hole diffusion coefficient
R_n is the net recombination rate for electrons
R_p is the net recombination rate for holes
G is the free carrier generation rate

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