Lead free Methyl-Ammonium Tin Iodide based Perovskite Solar Cells: Optimization of Perovskite Layer thickness through Simulation using gpvdm

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Introduction

- A perovskite solar cell is a solar cell which uses a material with perovskite structure as the light harvesting active layer.
- In the past few years organic lead halide perovskites based solar cells have been one of the most rapidly progressing solar cell technologies, with the efficiencies of these cells increasing from 3.8% in 2009 to 22.7% in late 2017 for single junction cells.
- These types of cells are of large commercial interest due to the potential of achieving much higher efficiencies as well as lower production costs due to the fact that they are solution processible.
- However, of primary concern is the introduction of the toxic material lead into the active layer of these solar cells, as well as the instability of these types of cells very moisture abundant environments.
- In order to combat the known issue of toxicity researchers have begun looking into tin, bismuth, antimony and copper chloride based halide perovskites.
- In this research we used the solar simulation software package gpvdm in order computationally maximize the efficiency of a tin based perovskite solar cell by optimizing the thickness of the active layer of the cell.

Methodology

Background and Theory of gpvdm

gpvdm (General-Purpose Photovoltaic Device Model) is general purpose solar cell simulation software package developed by Dr. Roderick MacKenzie of the University of Nottingham which is based on the solution of:

The Poisson Equation

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

Bipolar Drift Diffusion Equations

$$J_n = q\mu_c n\frac{\partial E_c}{\partial x} + qD_n\frac{\partial n}{\partial x}$$
$$J_p = q\mu_h p\frac{\partial E_v}{\partial x} - qD_p\frac{\partial p}{\partial x}$$

Carrier Continuity Equations

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

Where:
ε_0 is the permittivity of free space
ε_r is the relative permittiviry (Dielectric Constant)
φ is the voltage profile
q is the elementary charge of an electron
n is the free electron concenration
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 band edge
E_v is the free hole mobility band 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

The model solves the device equations in steady state or in the time domain, in 1D or in 2D. This model solves both electron and hole drift-diffusion, and carrier continuity equations in position space to describe the movement of charge within the device [1,2]. The model also solves Poisson's equation to calculate the internal electrostatic potential. Recombination and carrier trapping are described within the model using a Shockley-Read-Hall (SRH) methodology in which the distribution of trap sates can be arbitrarily defined [3].

Methodology

Simulation Setup

In Figure 2 we show the planar heterojunction architecture of a CH3NH3SNI9 (Methylammonium Tin Iodide) based perovskite solar cell. In this study we utilize the layer configuration Glass/Cathode/ETM/Perovskite/HTM/Anode (Back Contact). Hence we use FTO as our transparent cathode, TiO2 as an electron transport material (ETM), CH3NH3SNI9 as a perovskite, Cu2O as electron transport material and copper as a back contact anode.

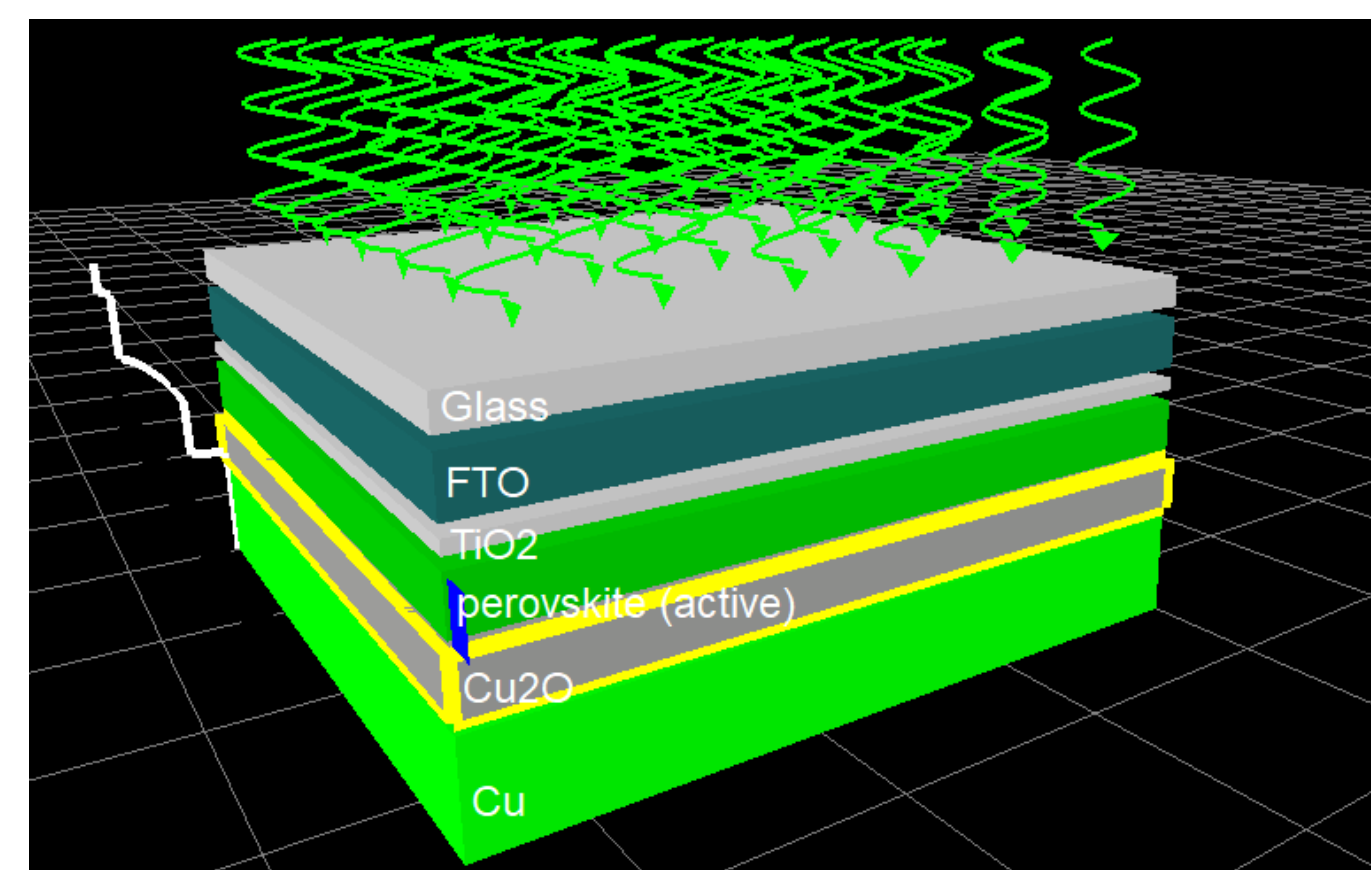In Table 1 we show the initial simulation parameters chosen from the gpvdm software database as well as [4] for $CH_3NH_3SNI_9$. The glass layer thickness was chosen to be $6(10^{-8})$m and the silver layer thickness $2(10^{-7})$m.

Figure 1. Planar heterojunction architecture of simulated cell (gpvdm)

In our study we look to obtain the effects of different layer thicknesses on power conversion efficiency. To do this we vary the layer thickness of each layer while keeping the other parameters constant. The initial layer thickness is given in Table 1 and is varied by 50 percent in each direction using evenly spaced points.

Table 1. Parameters used for Solar Cell Simulation

Parameters	FTO	TiO2	CH3NH3SNI9	Cu2O
Layer Thickness (m)	10^{-7}	$2.5(10^{-7})$	10^{-7}	10^{-7}
Relative Permittivity (ε_r)	3	9	8.2	7.5
Band Gap Energy	3.409	0.108	1.3	2.22
Electron Affinity (χ_i)	4.7	4.26	4.17	3.4
Electron Mobility [$m^2/(V.s)$]	$6.86(10^{-7})$	$20(10^{-4})$	$1.6(10^{-4})$	$3.0(10^{-3})$
Hole Mobility [$m^2/(V.s)$]	$3.75(10^{-2})$	$10(10^{-4})$	$1.6(10^{-4})$	$3.0(10^{-3})$
Donor Concentration (m^{-3})	$5(10^{-26})$	$1(10^{22})$	0	$2.93(10^{17})$
Acceptor Concentration (m^{-3})	$5(10^{26})$	0	$3.20(10^{15})$	0

Initial Simulation

From our initial parameters we obtain a power conversion efficiency of 10.8 percent, a fill factor of 0.731au and open circuit voltage of 0.694V and a short circuit current of -205 $A\,m^{-2}$. Figure 2 gives a plot of the Current Density vs Applied Voltage before optimizing layer thickness.
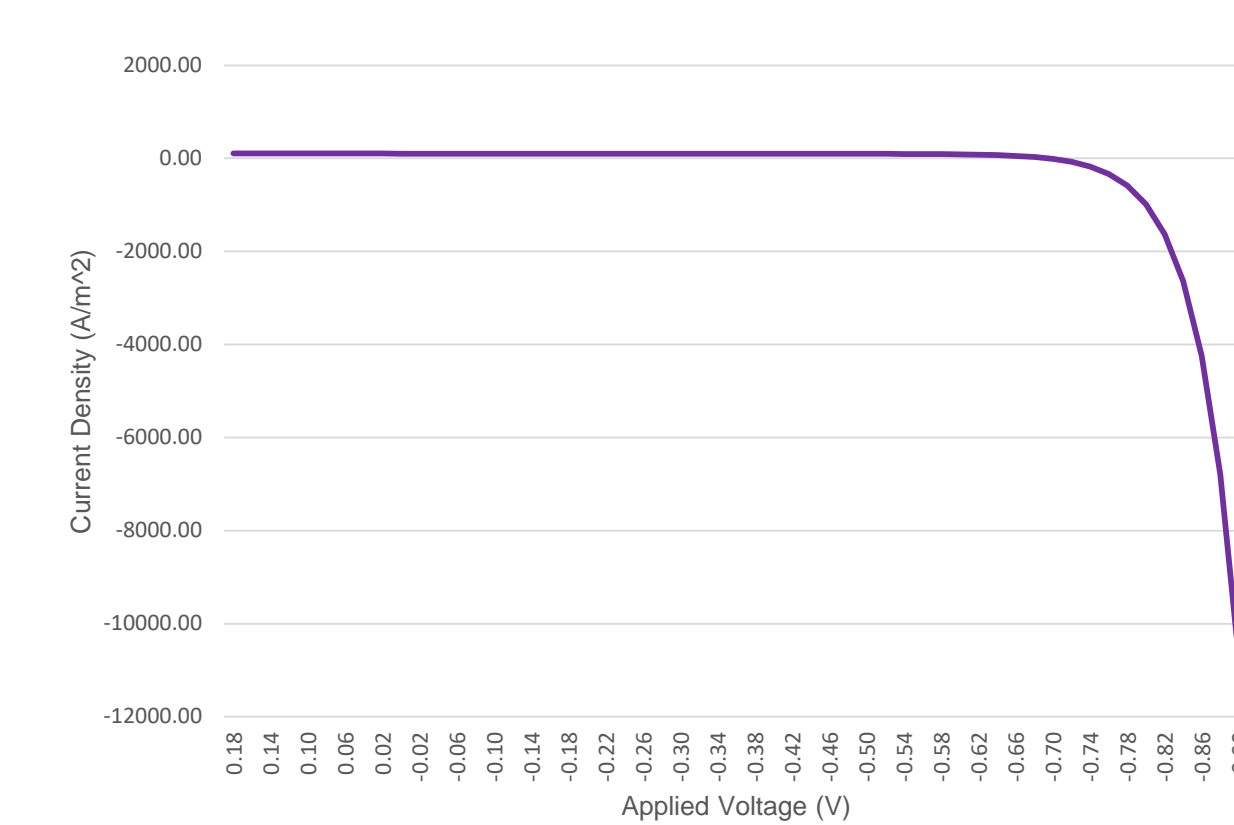
Figure 2. Current Density vs Applied Voltage before optimization.

Results and Discussion

Optimization of Power Conversion Efficiency

After simulation we obtained the data given in Figure 3. On our interval of thicknesses we are able to see a gradual increase in power conversion efficiency as the layer thickness increases with some minor drops at $9.44(10^{-8})$ m, $1.15(10^{-7})$ m, and $1.35(10^{-8})$ m, in an apparent pattern. The max power conversion efficiency was obtained at the right endpoint of the tested interval at $1.5(10^{-7})$ m. At this thickness we obtain a power conversion efficiency of 11.469 percent, a fill factor of 0.717au, open circuit voltage of 0.690 V and a short circuit current of -232 $A\,m^{-2}$. Figure 4 shows a plot of the current density vs applied voltage after optimizing the layer thickness for maximum power conversion efficiency.
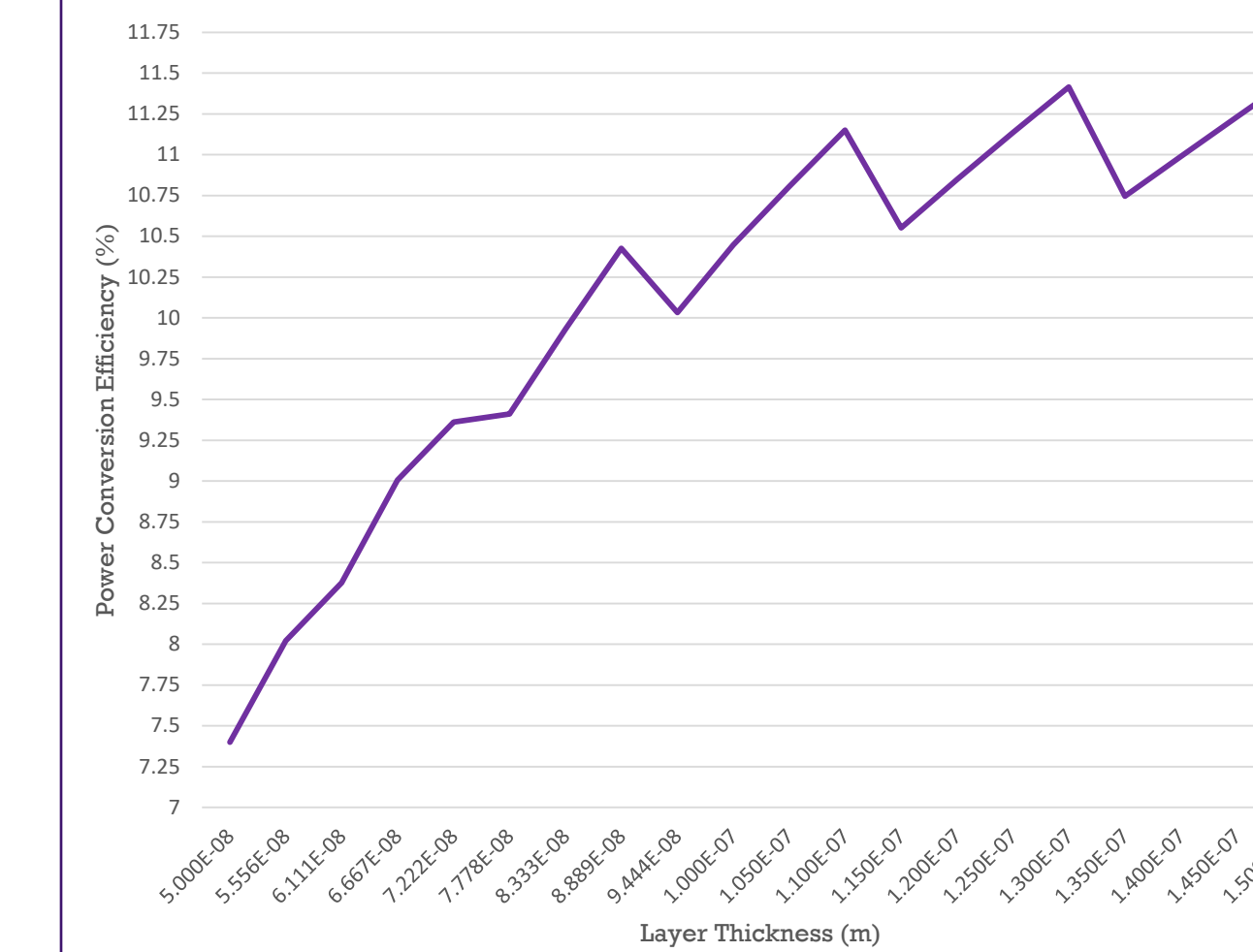

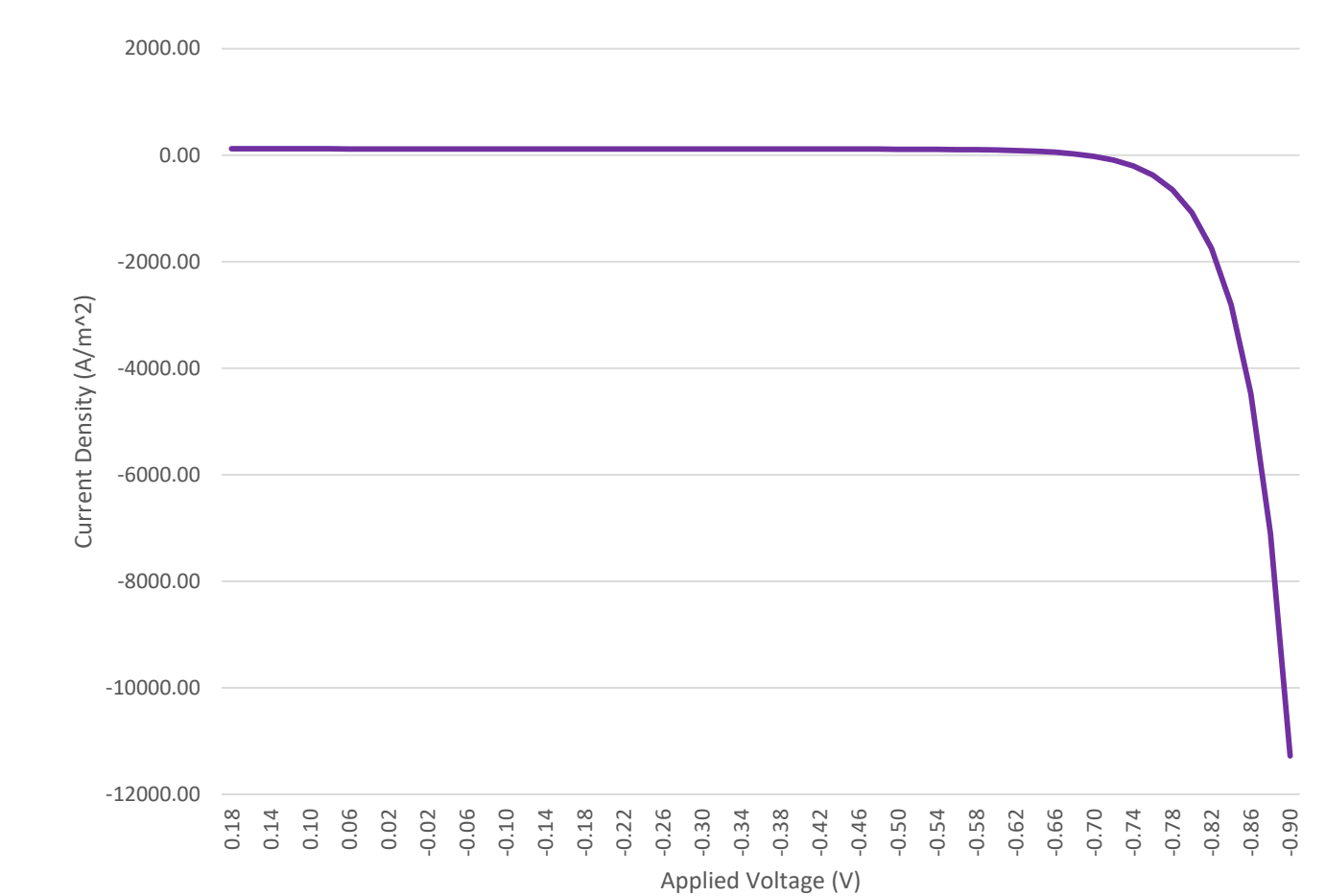**Figure 3.** Power Conversion Efficiency vs Layer thickness.

Figure 4. Current Density vs Applied Voltage before post-optimization.

Hence our simulations yielded favorable theoretical power conversion efficiencies for Tin perovskite cells which, in literature, show a maximum of around 10%. Also, by variation of the layer thickness of the perovskite layer we were also able to increase the power conversion efficiency of the cell beyond what was obtained by the initial parameters used.

Conclusions

- Within the simulated interval the efficiency of the solar cell was generally proportional to the thickness. However, there were significant drops at certain intermediate values.
- The obtained efficiency is lower than that of most lead-perovskite cells, but close to the around 10% max for lead halide perovskites.
- The max power conversion efficiency was found at $1.5(10^{-7})$ m, the right endpoint of the tested interval, with a power conversion efficiency of about 11.5 percent. This indicates that future work needs to be conducted on a wider spectrum of points in order to determine a more global trend for the efficiencies of this cell configuration.
- Further work will be conducted in order to understand how the optimization of the other non-perovskite layers affect the overall efficiency of the cell.

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