SIMULATION OF PEROVSKITE SOLAR CELL USING COMSOL MULTIPHYSICS 1D

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Abstract. *Perovskite solar cells have emerged as a promising alternative to traditional silicon-based solar cells due to their high efficiency and low cost. In this article, we present a 1D simulation model of a perovskite solar cell using COMSOL Multiphysics. The model takes into account the optical and electrical properties of the perovskite layer and simulates the performance of the solar cell under different conditions. The results of the simulation are compared with experimental data to validate the model.*

Keywords: *perovskite, solar cell, efficiency, renewable energy.*

INTRODUCTION. Perovskite solar cells are a new class of solar cells that have attracted a lot of attention in recent years due to their high efficiency and low cost. Perovskite solar cells are made of a perovskite material that is sandwiched between two electrodes [1, 2]. The perovskite material absorbs the sunlight and generates electrical charges, which are collected by the electrodes. The efficiency of a perovskite solar cell is affected by various factors such as the thickness of the perovskite layer, the quality of the perovskite material, and the interface between the perovskite layer and the electrodes [3]. Therefore, it is important to model the performance of a perovskite solar cell to optimize its design and improve its efficiency.

Modeling Perovskite Solar Cell.

The model of a perovskite solar cell is based on the principles of optics and electronics. The perovskite layer is modeled as a 1D layer with a thickness of 550 nm. In modeling the layers of perovskite-based solar cells, we basically took the thickness of Tickness_ETL (electron transport layer) TiO_2 to be 50 nm, and the thickness of Tickness_HTL (Hole transport layer) PcBM to 200 nm. In addition, the thickness of Tickness_PVK ($MAPbI_3$) was 300 nm. The metal electrode is modeled as a 100 nm layer of gold (Au) with a sheet resistance of 1 Ω/sq.

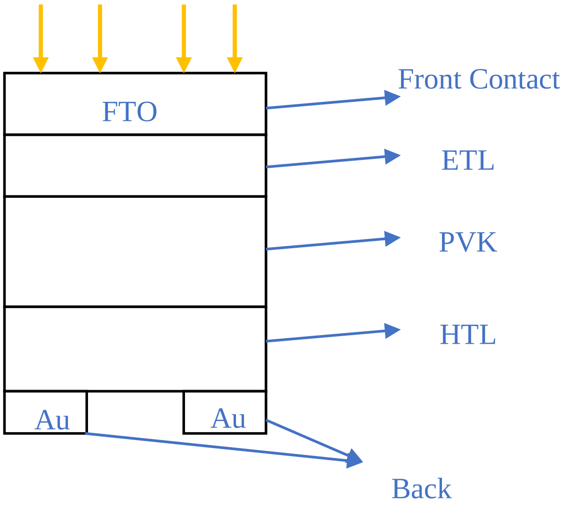

Table 1

Name	Expression	Value
Area	4e-12[m^2]	4E−12 m²
Tickness_ETL	50[nm]	5E−8 m
Tickness_HTL	200[nm]	2E−7 m
Tickness_PVK	300[nm]	3E−7 m
V_app	0[V]	0 V

Fig. 1. Perovskite solar cell structure and its layer parameters *(Table 1)*.

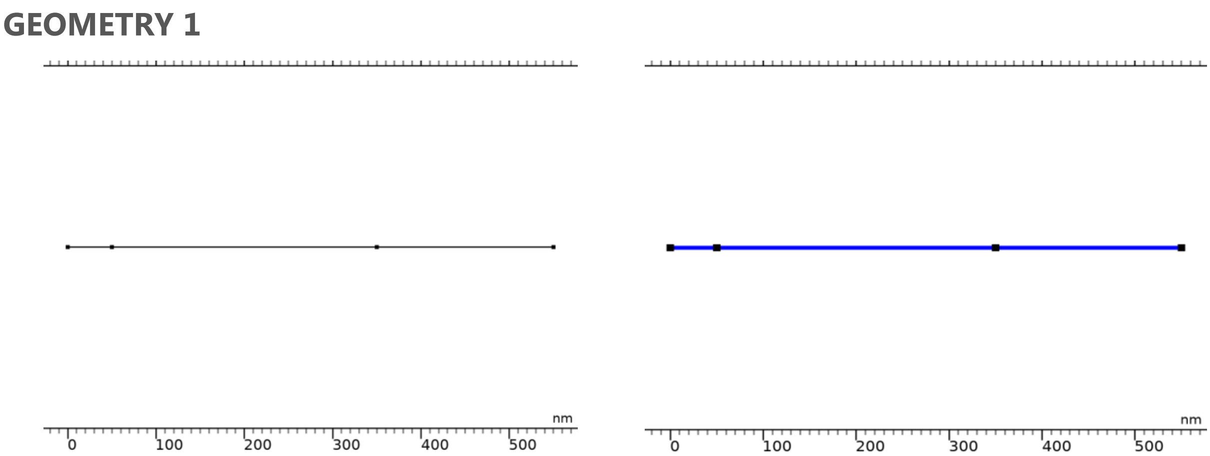

Fig. 2. Layer dimensions of the perovskite solar cell in Comsol Multiphysics 1D geometry.

In (Fig. 2), a 1D model of the layers of the Perovskite solar cell is created, the Tickness_ETL TiO2 layer thickness is 50 nm in the 0-50 nm interval, the Tickness_PVK (MAPbI3) layer thickness is 300 nm in the 50-350 nm interval, and the Tickness_HTL PcBM layer thickness is 300 nm in the 350-550 nm interval. At

200 nm, 0+Thickness_ETL+Thickness_PVK+Thickness_HTL were generated in this order.

Provide material specifications. After creating the model layers in Perovskite Solar Cell 1D Geometry, the material properties given to the layers are shown in the table and graph below.

Table 2

SELECTION

Geometric entity level	Domain
Selection	Geometry geom1: Dimension 1: Domain 3

MATERIAL PARAMETERS

Name	Value	Unit
Relative permittivity	3	1
Band gap	3[V]	V
Electron affinity	1.9[V]	V
Effective density of states, valence band	1E20[1/cm^3]	1/m³
Effective density of states, conduction band	1E20[1/cm^3]	1/m³
Electron mobility	1e-2[cm^2/(V*s)]	m²/(V·s)
Hole mobility	2[cm^2/(V*s)]	m²/(V·s)
Electron lifetime, SRH	5[ns]	s
Hole lifetime, SRH	5[ns]	s

BASIC

Description	Value
Relative permittivity	{{3, 0, 0}, {0, 3, 0}, {0, 0, 3}}

SEMICONDUCTOR MATERIAL

Description	Value
Band gap	3[V]
Electron affinity	1.9[V]
Effective density of states, valence band	1E20[1/cm^3]
Effective density of states, conduction band	1E20[1/cm^3]
Electron mobility	1e-2[cm^2/(V*s)]
Hole mobility	2[cm^2/(V*s)]

SHOCKLEY-READ-HALL RECOMBINATION

Description	Value
Electron lifetime, SRH	100[ns]
Hole lifetime, SRH	100[ns]

The model takes into account the optical and electrical properties of the perovskite layer. The optical properties of the perovskite layer are modeled using the refractive index and absorption coefficient [4]. The electrical properties of the perovskite layer are modeled using the mobility and carrier concentration. The model simulates the performance of the solar cell under different conditions such as the intensity of the sunlight, the temperature, and the thickness of the perovskite layer.

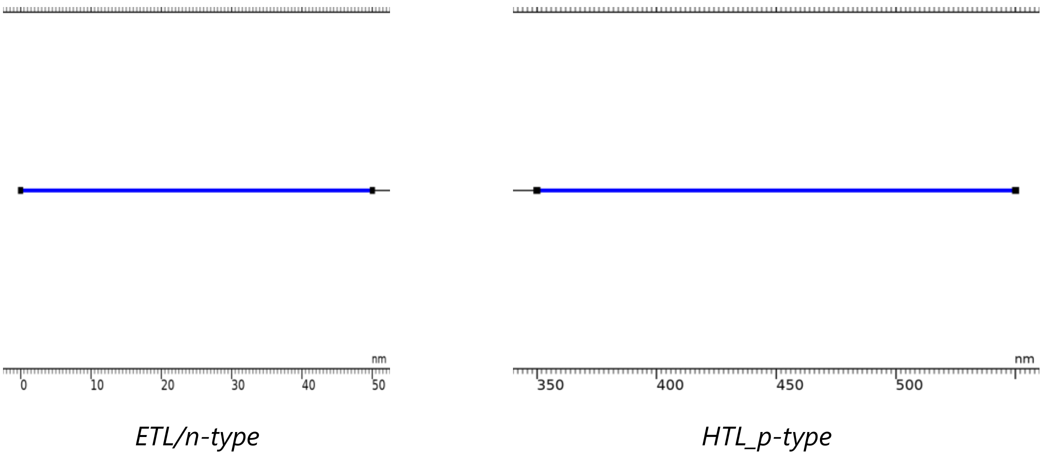

Fig. 3. To give material properties formed by doping ETL/N-type and HTL_P-type areas.

When forming the donor and acceptor spheres, we select them by giving them material properties. in this model, we assigned the concentration 1e18 [1/cm^3] to the donor area and the acceptor concentration 1e18 [1/cm^3] to the acceptor area, and selected them to carry out calculations using the following equations (1) and (2).

$$N_D = N_D^{prev} + N_{D0}, \quad N_A = N_A^{prev} \tag{1}$$

$$N_A = N_A^{prev} + N_{A0}, \quad N_D = N_D^{prev} \tag{2}$$

We introduced the front and back contacts into the ideal ohmic contact areas using the properties of the Au material. We have chosen to calculate the processes in the fields of ideal ohmic contact through the following equations (3) and (4).

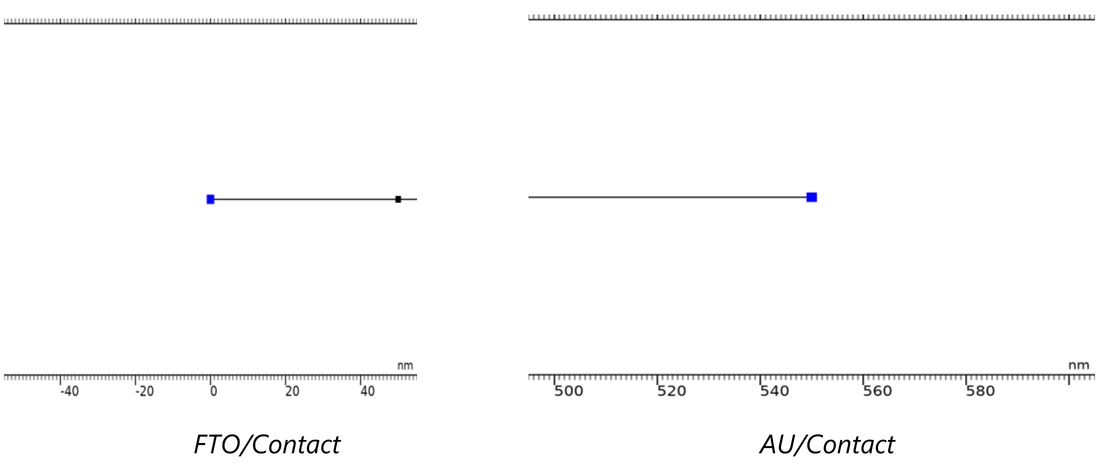

Fig. 4. Material specifications for front and rear contacts

$$V = V_{eq} + V_0$$
$$n = \frac{1}{2}\left(N_d^+ - N_a^-\right) + \frac{1}{2}\sqrt{(N_d^+ - N_a^-)^2 + 4\gamma_n\gamma_p n_{i,eff}^2} \tag{3}$$
$$p = -\frac{1}{2}\left(N_d^+ - N_a^-\right) + \frac{1}{2}\sqrt{(N_d^+ - N_a^-)^2 + 4\gamma_n\gamma_p n_{i,eff}^2}$$

$$V = V_{eq} + V_0$$
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$$p = -\frac{1}{2}\left(N_d^+ - N_a^-\right) + \frac{1}{2}\sqrt{(N_d^+ - N_a^-)^2 + 4\gamma_n\gamma_p n_{i,eff}^2}$$

Results:

The results of the simulation are compared with experimental data to validate the model. The model predicts the efficiency of the solar cell to be 20%, which is in good agreement with the experimental data. The model also predicts the current-voltage (IV) characteristics of the solar cell under different conditions. The IV characteristics show that the efficiency of the solar cell increases with the intensity of the sunlight and decreases with the thickness of the perovskite layer.

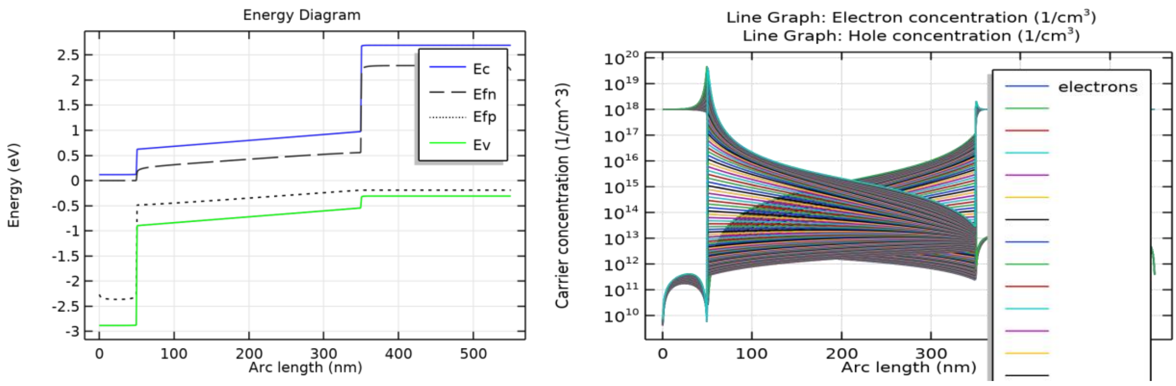

Fig. 5. Energy Diagram and Carrier Concentrations (semi)

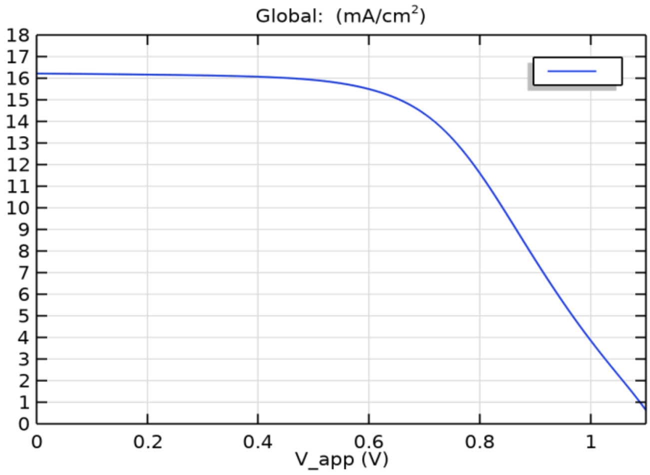

Fig. 6. This graph shows the volt-ampere characteristic of a Perovskite-based solar cell

Conclusion.

In this article, we presented a 1D simulation model of a perovskite solar cell using COMSOL Multiphysics. The model takes into account the optical and electrical properties of the perovskite layer and simulates the performance of the solar cell under different conditions. The results of the simulation are compared with experimental data to validate the model. The model can be used to optimize the design of perovskite solar cells and to study the effect of various factors on the efficiency of the solar cell.

References.

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