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Original Article

Effects of Thickness and Defect Material on Perovskite Solar Cell Efficiency

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Abstract - *This work aims to investigate the effects of two parameters on a solar cell with perovskite as the absorption material. As the natural energy resources are available in abundant quantity on earth, the cost of utilizing these resources is less compared to the cost of fossil fuels like petrol, diesel, and similar non-renewable energy sources. There is a need to identify, utilize and enhance the performance of renewable energy sources. Renewable energy is a source of pure, limitless, and increasingly abundant energy. They vary from fossil fuels in their diversity, quantity, and their use anywhere on the earth. They do not emit greenhouse gases and do not cause pollution. Solar energy is obtained from the sun's radiation. These Radiations are converted to electricity, and this electricity is used for home and industrial purposes. This research examines the performance of a perovskite-based solar cell by varying the thickness and defect density of the material. The efficiency of the cell is calculated based on the variation of Defect density and thickness. The thicknesses of the layers varied, and accordingly, efficiency was calculated. Efficiency is reduced to 24.84% when defective material is added to the current construction. When the absorber layer's thickness is changed from 0.03 to 0.09 μm, efficiency rises to 34.24%. The recorder shows the waveforms between the efficiency and the thickness of different layers. The simulation of a perovskite solar cell is done using the SCAPS 1D simulation tool.*

Keywords - *Solar energy, Energy dissipation, Fuel cells, Solar cell, Energy efficiency.*

1. Introduction

The weather changes significantly due to increased global warming, which has an impact on the environment. Energy conservation, or the preservation of natural resources, is required to stop this change in the weather. Electricity is generated at power plants using coal and other fossil fuels. This results in a high level of pollution from power plants. Air pollution causes the release of various poisonous gases, including carbon dioxide, which is harmful to humans and to the environment. Hence, Air Pollution must be reduced to stop global warming. The solution to this is the utilization of natural resources, which allows us to produce energy while protecting the environment.

This outlines the need for solar cells. That is the generation of electricity from solar cells with the help of natural resources. The natural resource that humans may easily access is sunlight. Solar cells absorb this sunlight. Solar cells transform solar radiation into the electrical power required for our habitation. Automobiles are also capable of running on electricity. There are two types of energy available to human beings. The first one is renewable energy, and the second is non-renewable energy. Renewable energy is the energy that cannot be exhausted as we utilize it. Some examples of renewable energy that are available to us are solar energy and wind energy.

Non-renewable energy is derived from resources that cannot be replenished, including coal, oil, natural gas, and fossil fuels. These non-renewable energy sources have several disadvantages. As indicated by global temperature data that has been published [1], there has been a rise in global warming due to temperature fluctuations and the emission of harmful gases. This illustrates the impact of non-renewable energy sources on global warming. Furthermore, the projections for future temperature changes suggest a further increase in global warming.

Due to the production of non-renewable energy sources, particularly oil drilling, coal mining causes significant land degradation, increases pollution and damages to habitat. Due to the obvious disadvantages of non-renewable energy, it is vital to use resources that are readily available in nature. The solution is to employ renewable energy. Renewable energy emits no greenhouse gases from fossil fuels and minimizes air pollution.

Over the next several years, the demand will rise in tandem with population expansion. Renewable energy is in increasing demand for cars, which necessitates research into the use of plentiful resources to meet this demand. Vehicles use diesel or petrol, which is manufactured using non-renewable energy. Additionally, the cost of producing this electricity is lower. As a result of various downsides, this energy is being replaced with renewable energy sources. A major source of renewable energy is sunlight. Therefore, it is necessary to use solar panels to create solar cell structures. These solar cells absorb sunlight and generate electrical energy using photovoltaic technology. This solar energy has higher efficiency and longer service life.

The structure of a solar cell consists of a Hole Transport Layer (HTL), an Electron Transport Layer (ETL), glass (FTO), and an absorption layer. The absorption layer acts as a semiconductor that captures photons, exciting electrons into the conduction band and generating photocurrent. Various semiconductor materials are utilized as absorption layers depending on their efficiency and longevity. These materials include copper, indium, gallium, and selenium. Currently, much of the research is focusing on perovskite materials due to their high efficiency and extended lifespan. The research presented in this paper is centered on the application of solar cell structures that use perovskite as the absorption material.

In this paper, perovskite is used as an absorption material due to its higher efficiency. The chemical formula of a solar cell is a combination of ABX3. Where A is a cation that is divalent, B is a metallic cation that is tetravalent, and X is a halide ion (Cl, Br, I). Lead-based Perovskite solar cells have an efficiency greater than 30% [2] by varying defect density, thickness, and temperature using SCAPS. The efficiency of lead-based solar cells also improved by using an inverted heterojunction structure, i.e., by changing illumination from right to left [3]. Device modeling of solar cells is performed using CH3NH3PbI(3-x) Cl3 as absorption material [3]. They studied how the diffusion length of carriers in the absorber correlates with the defect densities at the front and back interfaces. By utilizing perovskite as the absorber material, they attained efficiencies exceeding 15%. The device simulator SCAPS3309 is used for the simulation of materials. The researchers [4] proposed a modelling technique for perovskite solar cells based on their structural similarities to thin-film inorganic semiconductor solar cells.

Perovskite solar cells' electrical characteristics, including their efficiency, fill factor, open-circuit voltage and short-circuit current, are investigated. Mathematical equations [5] for simulating the performance of polycrystalline semiconductor solar cells under various conditions, such as changing sunlight intensity, temperature, and material parameters, are developed. The implications for enhancing the efficiency and reliability of polycrystalline semiconductor solar cells are explored. A perovskite solar cell architecture with a thin insulator layer of TiO2 for efficient electron transport has been created and characterized [6]. The way solar cells behave in various temperature and sun exposure scenarios is explained [7]. The performance of solar cells is investigated using a physics-based analytical model that considers critical factors. The best design parameters are derived by taking into account two primary PSC structures: p-i-n and n-i-p [8]. A unique numerical technique for solving models of charge carrier transport and ion vacancy migration in perovskite solar cells is provided [9]. The electrical performance of inverted planar perovskite solar cells is simulated using different configurations of metal oxide transport layers. The thickness, composition, and interface properties of the transport layers are optimized to improve device performance. The study may have investigated the effects of different metal oxides, such as TiO2, ZnO, and SnO_2, on charge transport and recombination [10]. Simulated optoelectronic characteristics of a monolithically integrated terminal tandem solar cell are examined, with particular focus on the impact of a silicon tunnel junction. The tandem cell is anticipated to have a maximum efficiency of 27% [11].

The process of developing PSCs from discovery to laboratory research to commercialization is reviewed. The materials utilized in perovskite solar cells, production procedures, performance measures and possible applications are reviewed [12]. Perovskite solar cell review and advances in the various perovskite solar cell implementation are presented [13], and different fabrication routes are elaborated [14]. Performance parameters are observed for a free solar cell [15]. Tin, carbon, and polymer-based Perovskite cell working, advantages, and disadvantages are described [16].

The efficiency of solar cells achieved is 15.1% with the help of a polyaniline layer [12]. A detailed review of the perovskite solar cell is given in [17]. The efficiency of a perovskite solar cell differs depending on the composition of its components [18, 19]. Natural light energy obtained from sunlight is abundant and readily available to us. Perovskite solar cells are less expensive and have higher efficiency. This is a new emerging technology, and most researchers are aiming to achieve improved efficiency while keeping costs low [20].

Various device structures are investigated, and their performance factors are calculated [21]. The effects of defect density are evaluated using SCAPS [22]. The efficiency of a solar cell with an inverted configuration is 24.83% [25]. Simulation software is used to investigate the effect of absorber layer properties on performance parameters using p-i-n [23], n-i-p [24, 29, 36] structure, lead-free perovskite [30, 32, 33], and CZTS [31]. Various structures of solar cells are investigated using SCAPS software [26, 27, 28], and performance parameters [37, 38, 39] are evaluated. The performance of the solar cell is also investigated with and without the HTL layer [34].

This paper is organized as follows. Section 2 outlines the problem formulation, describing the importance of research in the area of solar cell material. Section 3 outlines the materials and methods employed to enhance the efficiency of Perovskite Solar Cells (PSC). Section 4 presents the results and discussion concerning the solar cell.

2. Problem Formulation

Because of the extraordinary conversion efficiency of its next-generation photovoltaic technology, perovskite solar cells are leading the way in the solar battery revolution. This is a rapidly growing field with extensive new research underway. These cells are cost-effective, and their chemical composition is straightforward. It is clear from reviewing research studies on perovskite solar cells that additional investigation in this area is essential. There is potential to alter more material characteristics, and the performance metrics are currently being explored. Identifying the performance factors that yield the highest efficiency and longevity for solar cells is crucial. Thus, further research into perovskite solar cells is necessary.

3. Materials and Methods

A solar cell has a p-i-n configuration. The main charge carriers in an N junction are electrons. The bulk charge carriers in the P junction are holes. Sunlight gives Photon energy. Through an N junction, this photon energy enters the depletion area where it creates electron-hole pairs, which in turn produce an electric current. SCAPs is a solar cell simulator software developed at University of Gent, Belgium. Perovskite is simulated between three layers. The first layer is the Hole Transport Layer (HTL), the second layer is the perovskite, i.e., the absorption layer, and the third layer is the Electron Transport Layer (ETL). In SCAPs, illumination is changed from dark to light because, for stability, simulations are done in light only. AM1.5 G1 sun spectrum is selected. There is an organic-inorganic type of Perovskite Solar Cells (PSC). Different structures are proposed for Perovskite solar cells by changing materials and their characteristics. By varying their structure, the efficiency is calculated. CB effective density of states and VB effective density of states (1/cm3) parameters are calculated by the continuity equation and Poisson's equation. Important parameters on which the performance of a solar cell depends are FF, efficiency(eta), Jsc, and Voc. Equation (1) and Equation (2) gives the relation between important parameters of the cell. Most of the researchers tried to increase the efficiency of solar cells by varying material parameter values. Various materials can be used to increase efficiency. Many factors affect efficiency changes. Some of the factors contributing towards increasing efficiency are bandgap voltage, electron affinity, defect densities, temperature, thickness, work function and electrical properties of solar cells. To increase the efficiency of solar cells, Jsc, Voc, and FF parameters are to be increased. In the simulation of Solar cells, the effect of sheet and shunt resistance is not considered. AM1.5G, i.e. Air Mass 1.5 Global SUN is used for simulation. This consists of 1000 W/m^2 of power. Bandgap voltage is considered low because if the bandgap voltage is increased, then the distance between Ec and Ev layers is increased, and less recombination occurs, which results in a decrease in efficiency.

$$FF = \frac{Pmax}{JscVoc} \tag{1}$$

Where FF= Fill Factor, Pmax=VmaxJmax,

$$Voc = \frac{kT}{q} ln\left[\frac{Jsc}{J0} + 1\right] \tag{2}$$

$$eta = \eta = \frac{JscVocFF}{Plight} \tag{3}$$

J0 is the Saturation current density, kT/q is the thermal voltage for 3000 K. Jsc is the short-circuit current density. Voc is the open circuit voltage.

Many research studies show simulation results of different materials, and the analysis is based on the comparison of Voc, Jsc, FF, and eta. The basic structure of Perovskite consists of a Hole transport layer, an Absorption layer, and an Electron transport layer. Many studies have been carried out using different HTL and ETL layers, and efficiency and other parameters have been calculated. Figure 1 gives the schematic of Perovskite based solar cell with an FTO layer. In this schematic, four layers are used between the left and right contacts, and Cu2O material is used as the HTL layer. TiO2 material is taken as the ETL layer. Perovskite material is CH3NH3Pb(1-x)Clx. Two interfaces are used in this structure. One interface is between HTL and perovskite material, and the second interface is between Perovskite and ETL layer. Illumination of the light path is from the right contact to the left layers, as shown by the arrows. The left side of Figure 1 shows a stack of layers from left contact to right contact using an FTO layer. Various Interfaces used between the layers are also given. The right side shows a pictorial representation of these layers.

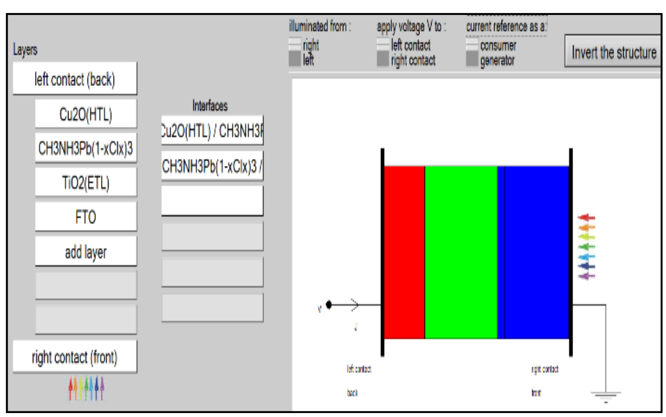

Fig. 1 Schematic of perovskite based solar cell, including the FTO layer

Table 1. Material properties of all layers

Parameters	Cu_2O (HTL)	CH_3NH_3Pb (1-xClx)3	TiO_2 (ETL)	FTO
Thickness (um)	0.250	0.450	0.040	0.400
Band gap (eV)	2.170	1.550	3.200	3.500
Electron Affinity (eV)	3.200	3.930	3.900	4.000
Relative Dielectric Permittivity	7.110	6.500	9.000	9.000
CB effective density of states (1/cm^3)	2.020E+17	2.200E+17	1.000E+21	2.020E+18
VB effective density of states (1/cm^3)	1.100E+19	1.800E+19	2.000E+20	1.800E+19
Electron thermal velocity (cm/s)	1.000 E+7	1.000 E+7	1.000 E+7	1.000 E+7
Hole thermal velocity(cm/s)	1.000 E+7	1.000 E+7	1.000 E+7	1.000 E+7
Electron mobility (cm^2/Vs)	2.000E+2	2.000E+1	2.000E+1	2.000E+1
Hole mobility (cm^2/Vs)	8.000E+1	2.000E+1	1.000E+1	1.000E+1

In this representation, the red color shows the Cu2O material layer. Green color is the middle layer, which is taken as the Perovskite layer, and blue color shows the ETL layer. As the FTO layer is added, the width of the ETL layer is increased. Different properties of materials used here are given in Table 1. FTO is the glass material. Parameters of FTO are taken from the research paper [23].

4. Results and Discussion

When the beam of sunlight hits the silicon material, photons or light energy are absorbed, reflected, and transmitted. When a photon is absorbed in the absorber layer, it transfers energy to an electron, forming an electron-hole pair. These electron-hole pairs move in opposite directions, resulting in the flow of electric current. Two different outcomes are discussed in this section. The initial performance parameter findings are noted both with and without the addition of defect material to each layer. The influence of thickness variation on cell performance parameters is also evaluated.

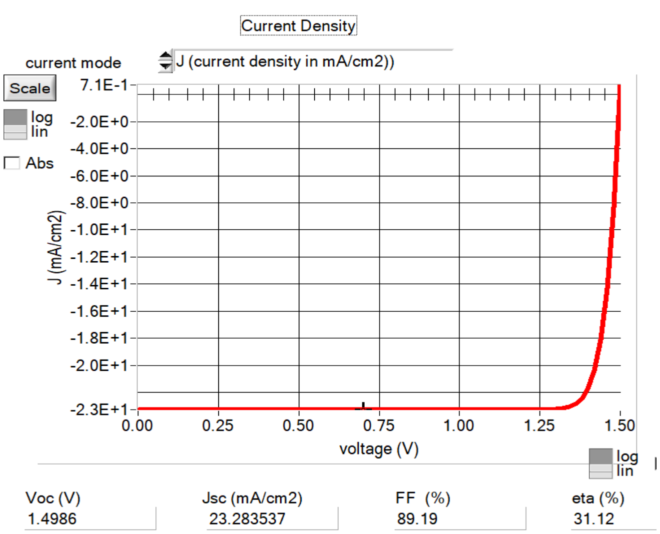

Fig. 2 I-V characteristics of a solar cell without adding defect material

4.1. Effect of Defect Material

Two types of simulation parameters are considered when calculating the performance parameters of a solar cell. In the first case, parameters are observed by taking all the layers without adding defect material. Figure 2 shows I-V characteristics using a batch analysis simulation of a solar cell without adding defect material to the layers. This gives an efficiency of 31.12%. Short circuit current increases to 23.28 mA/cm^2 after a voltage of 1.25 V

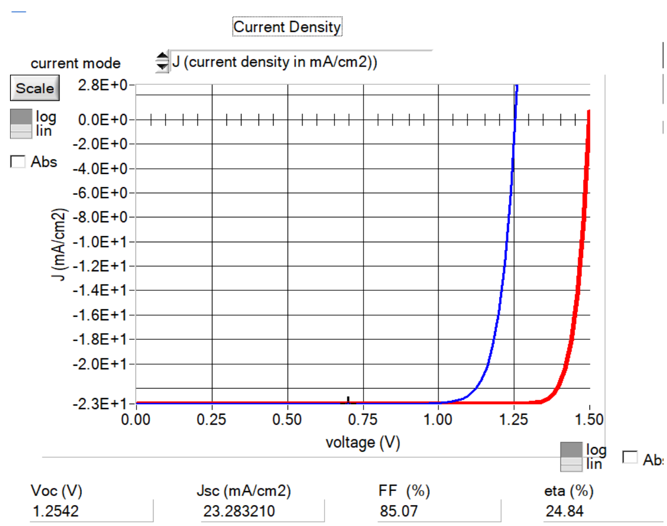

Fig. 3 I-V characteristics of a solar cell by adding defect material

Figure 3 shows the I-V characteristics after adding defect material. Adding defect material to each layer decreases efficiency to 24.84% with a decrease in open circuit voltage of 1.2542V. Table 2 summarizes the effect of adding and not adding defect material. As the defect density is reduced, efficiency is increased. The lifetime of the carriers is shortened when the density of defects rises, along with the recombination rate. Trapping them quickly leads to increased recombination and decreased cell efficiency, as shown in Table 2. Defect density is reduced and efficiency is increased.

$$\tau_{n,p} = \frac{1}{\sigma_{n,p} v_{thn} N_t} \quad (4)$$

$\sigma_{n,p}$ are the capture cross section of charge carriers, vthn is the velocity of charge carriers, and Nt is the absorber layer defect density. Carrier lifetime is inversely proportional to defect density, as shown in equation 4. Addition of defect density increases recombination rate and decreases efficiency.

Table 2. Effect of defect material on performance parameters

Parameter	Efficiency	FF	Voc	Jsc
Without adding defects	31.12	89.19	1.4886	23.28
Adding Defects	24.84	85.07	1.2542	23.283202

4.2. Effect of Thickness Variation

In this, the thickness of the layers is varied, and efficiency is observed. Thickness is varied using a batch analysis setup. All three layer thickness parameters are set in the range given in Table 3.

This table gives the values of performance parameters for thickness variation.

Table 3. Variation in thickness

Range of Thickness Variation for Basic Layers	Efficiency (%)	FF (%)	Voc (V)	Jsc (mA/cm^2)
ETL layer thickness is varied from 0.03 um to 0.08 um	31.06	89.19	1.4986	23.239640
The thickness of the HTL layer is varied from 0.250 to 0.65 um	31.22	89.19	1.4988	23.352576
The thickness of the Absorber layer is varied from 0.03 to 0.09 um	34.24	89.12	1.5027	25.569030

Efficiency is decreased if the thickness of the ETL layer is varied from 0.03 um to 0.08 um, then the efficiency is decreased from 31.12% to 31.06%, as shown in Figure 4.

Similarly, efficiency is observed by changing HTL and Perovskite layer thickness. Efficiency is increased to 34.24% if the absorber layer thickness is varied from 0.03 um to 0.09 um.

Variation in the thickness of HTL, Perovskite and ETL layers is done, and efficiency is observed. Figure 5 gives the surface plot of Table 3 for thickness variation.

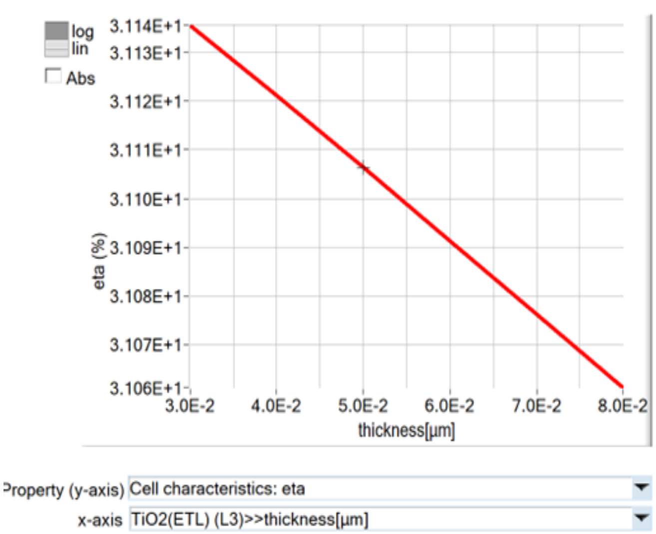

Fig. 4 Thickness variation of ETL Layer

Figure 5 shows the graphical representation of the thickness variation of three layers. It can be seen from the above results that, by varying the absorber layer thickness, efficiency is increased. Thickness variation has a greater impact on the efficiency parameter than the defect density parameter.

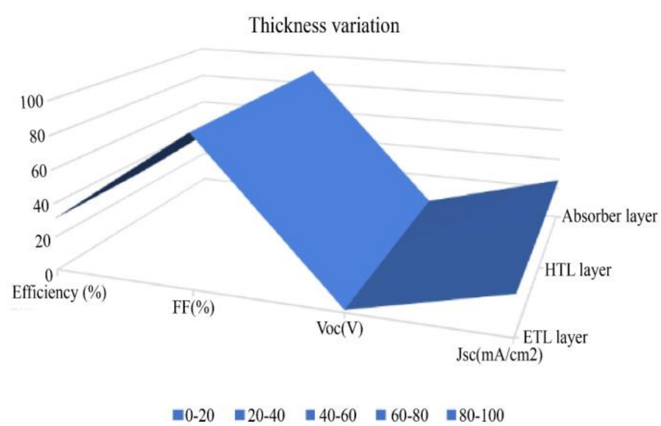

Fig. 5 Surface plot of ETL, HTL, and absorber layer thickness variation

Table 4 shows the comparative analysis with [23]. [23] used NiOx-Perovskite-ZnO cell structure. It can be seen that the efficiency of Cu_2O -Perovskite-TiO_2-FTO structure is higher compared to the [23]. This gives the results of adding defect materials.

Table 4. Comparison with existing work [23]

Structure	Efficiency (%)	FF (%)	Voc (V)	Jsc (mA/cm2)
NiOx-Perovskite-ZnO [23]	22.48	50.75	1.388	31.903
Cu_2O-Perovskite-TiO_2-FTO (This work) with adding defects	24.84	85.07	1.2542	23.283202

Table 5 compares the thickness variation with other available structures. Results obtained from three structures are taken for comparison. It is observed from the table that the efficiency of the Perovskite-based solar cell is higher than that of CZTS and the lead-free structure. Hence, perovskite-based solar cell is the most preferable solar cell technology.

Table 5. Variation in thickness

Range of Thickness Variation for Basic Layers	Efficiency (%)	FF (%)	Voc (V)	Jsc (mA/cm2)
[30] CZTS structure	31.86	83.37	1.19	32.05
[31] lead-free perovskite	30.19	87.33	1.1	31.42
Thickness of the Absorber layer is varied from 0.03 to 0.09 um (This work)	34.24	89.12	1.5027	25.569030

5. Conclusion

This paper analyses solar cell efficiency using perovskite material as an absorber layer. The hole transport layer used is Cu2O, and the Electron transport layer is TiO2. The material properties of these layers are set in Table 1. The effect of Defect material is determined using a batch analysis setup. Efficiency is decreased to 24.84% after adding defect material. The thickness of ETL, HTL, and the absorber layer is varied, and performance is analyzed. The thickness of the absorber layer gives a sufficient increase in efficiency to 34.24%. The thickness of the absorber layer variation increases efficiency as compared to the defect density parameter.

Performance parameter decreases with the addition of defect density and increases with thickness variation. This structure is compared with other available structures. Based on the comparison structure, using the Perovskite material gives more efficiency than other available structures.

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