Design and Simulation of PEDOT: PSS and P3HT: PCBM based HIT Solar Cell to Improve the Internal Quantum Efficiency

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Abstract - *Meticulously consumption of Energy is the tremendous field for the growth and development of mankind. Researchers all around the world are finding new ways to explore the maximum utilization of renewable energy in one form or the other. The photovoltaic modules are best to date of technology which converts solar energy to usable form. This paper deals with the design of photovoltaic cell with better efficiency and Fill Factor and its usage as a case study that describe the generation and installation estimation of power for Shimla city. The design of rooftop solar panel power generation is done numerically and an estimation for city planned by using data provided by Town and Country Planning Department, Shimla, Govt. Of Himachal Pradesh. The design and simulations are performed using SCAPS and Comsol 5.4 (Student Version).*

***Key Words*: Photovoltaic cell, Form Fill Factor, Quantum efficiency, Heterojunction intrinsic thin layer solar cell, Saturation current, Solar grid.**

1.INTRODUCTION

The creed of technology race is declining the non-renewable energy resources of the globe and affecting its stability towards environment and nature. And this is attracting the researchers' interest to utilize renewable resources available on the earth. The extraction of electricity out of solar energy using photovoltaic module is the best suited methodology till date. In the past few years, number of researchers around the globe have designed and tested many different solar cells to increase the conversion efficiency of solar energy to electricity. Different materials, shapes, structures and methodologies have been developed by numerous researchers to achieve maximized efficiency. Semiconductor materials with finite bandgap energy are best possible choice for the researchers. Silicon (Si) is an abundant element available on earth and show its dominance in designing solar material. Its low toxicity towards solar radiation and low cost for large deployment makes its best suited materials for photovoltaic cell. However, it has an indirect bandgap of with bandgap energy of 1.1 eV that presents limitation towards optical absorption. The efficacy of the solar cell determines through its conversion capability of incident light to electric power with small electrical losses. So, to design an efficient solar cell the consideration of optical and electrical aspects are taken care of. To enhance the conversion efficiency the optical path length is so designed such that the incident light can remian in light absorber for longer period of time. Howevevr, to minimize the electric loss the short collection length is the necessasity of effective collection of photogenerated carriers to recombine. The silicon heterojunction (SHJ) solar cells gain the prime concern of of community researchers due to their simplicty in fabrication, ease in operation, better perfofrmance and reduced temperature coefficient. It have the limitation of absorption of incident light. Whereas, researchers have developed the appraoches to improve incident light absorption through textured structures, periodic gratings, photonic crystals, and nanostructure arrays. These patterned silicon cells enhances the light absorption efficiency but complexes the electrical design as recombination of photogenerated carriers take place which reduces the photovoltaic effect and that results to degraded effeiciey of these patterned Si cells.

With limitless demand of energy and changes in climatic conditions, photovoltaic cells are gaining popularity in the world's renewable energy consumption sectors. The progress in developing of new solar cell technologies with reduced production costs is therefore of great interest to industry. The intensive research is under progression to develop new, prospective materials in order to manufacture reduced cost and efficient photovoltaic devices with different compositions such as organic, hybrid organic-inorganic, and inorganic heterojunctions. Their unique properties with different material evolve new scope to improve the operational and design characteristics of heterojunction solar cells with intrinsic layer. The advantage of HIT solar cells over crystalline solar cells is that it can be fabricated under low temperature (~ 200-300°C). This allows the cells to be made on the silicon wafer of about 70nm in thickness without destroying it (Yang et al., 2019). The low temperature process reduces the energy need for production, thereby reducing the energy payback time and increasing the beneficial effect of photovoltaics on the environment.

To improve the efficiency of the panel heterojunction solar cell made up of different materials are simulated using software COMSOL 5.0 and GPVDM 2.0. To produce the solar based electricity a plan is proposed for the rooftop areas available in Shimla city to setup production house for solar energy-based grid in future. Different techniques and methodologies used to develop thin films of the solar cells.

These include molecular beam epitaxy, Liquid Phase Epitaxy, Chemical Compound Based Solar Cell. This research paper is organized as: Section I is describing the Introduction followed by, Section II which details about the basics of HIT Solar cell. The section III elucidates the parameters and methodology to design the solar cell and rooftop planning of the solar panel installation. Section IV explain the simulation results and discussion followed by Conclusion.

2. HETERO-JUNCTION INTRINSIC THIN LAYER SOLAR CELL

The hetero-junction composition of thin layer is the amalgamation of amorphous silicon and crystalline silicon technology. This results into a heterojunction with intrinsic thin layer (HIT) solar cell. The HIT solar cell has exclusive features which include, high conversion efficiency and low processing temperature, that makes it best suited for large scale commercialization and substitute for traditional source of power.

The procedure of fabrication of HIT solar cells is less complicated as compared to other, the crystalline silicon, firstly the c-Si cell is fabricated, which is trailed by deposition, a-Si:H (intrinsic type) and extrinsic amorphous silicon, n-type and p-type a-Si: H.

The deposition is done through plasma enhanced chem1ical vapor deposition (PECVD) that is comparable to fabrication process of thin-film. Currently only n-type c-Si wafers are used to manufacture commercial HIT solar cells but some researchers focusing on HIT solar cells made of various kind of compounds/organic compounds.

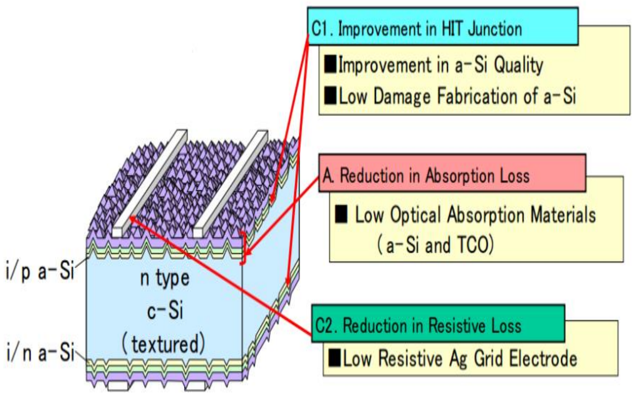

Figure 1. Key features of HIT Solar Cell

The fabrication process of HIT solar cell is cheaper and simpler as compared to other processes. The popularity of HIT solar cell is due to its low process temperature (~ 200°C), as compared to crystalline silicon (c-Si) solar cell (nearly 1000°C) and relatively high efficiency, η (capability of reaching efficiency up to 29%) (Gray & Durbin, 1994). The other interactive feature of HIT solar cell is its better stability under light, less dark current that means high efficiency even in limited space and light. The materials used for fabrication are less costly and abundant in nature. The exceptional passivating property of the a-Si:H(i) increases the V_{oc}, which then result to an improvement of the short I_{sc} and FF.

3. PARAMETERS DESCRIPTION AND DESIGN METHODOLOGY

The basic parameters which describe the characteristics of solar cell are V_{oc}, I_{sc} and FF means open circuit voltage, short circuit current and Fill Factor respectively. The V_{oc} can be evaluated by equating resultant current to zero in solar cell equation given as:

$$V_{OC} = \frac{\eta kT}{q}\, In\left(\frac{I_l}{I_0} + 1\right) \quad ....(1)$$

This equation elucidate that V_{oc} depends upon the saturation current (I_o), which ultimately depends upon the recombination of charge carriers at the junction of the solar cell. Hence, open circuit voltage points to amount of recombination in the photovoltaic cell. Here, k is boltzmans constant, T is absolute temperature and q represents the charge.

The I_{sc}, is short circuit current defined as short circuit current density (J_{sc}) times the exposure area of the cell. The J_{sc}, short circuit current density varies as per the surface area of the solar cell exposed to the incident light and intensity of of photons, the spectrum of incident light such that follows the Planck's law and absorption probability of the incidnet photons. The expressions are given as:

$$J_{sc} = qG(L_n + L_p) \quad ....(2)$$

$$I_{sc} = J_{sc}\, A \quad ....(3)$$

The maximum power generated by a solar cell can be analysed through fill factor (FF). It depends upon Voc and Ioc. The expression for FF can be given as:

$$FF = \frac{V_{MP}\, I_{MP}}{V_{OC}\, I_{SC}} \quad ....(4)$$

$$P_{max} = V_{oc}\, I_{sc}\, FF \quad ....(5)$$

$$n = \frac{P_{max}}{P_{in}} \quad ....(6)$$

3.1 IMPLEMENTATION DETAILS

Energy is backbone for the growth of mankind and it require a careful usage and conservation. The solar energy can be employed to lighten up the homes, industrial manufacturing and processing, and other applications. The only basic requirement is its generation and proper storage for in future use. The application study is done in this chapter where a brief layout is discussed and designed for ON GRID solar panel installation. In this chapter we discussed about design procedure of rooftop solar power generation setup.

A solar cell with dimensions of few centimeters can generate very little electrical power. The commercially available solar cell unit of dimensions 12 cm × 12 cm generates about 3 watts of electrical power based on 18-20 percent of solar energy incident on it. To boost the voltage these cells are connected in series or in parallel they increase the output current. The conversion efficiency of solar cells is different as per their fabrication and architecture. A monocrystalline solar cell is much more efficient as compared to polycrystalline solar array. The fabrication of solar panels are generally made up of 36-56 interconnected cells which are fitted with lamination inside an aluminum frame.

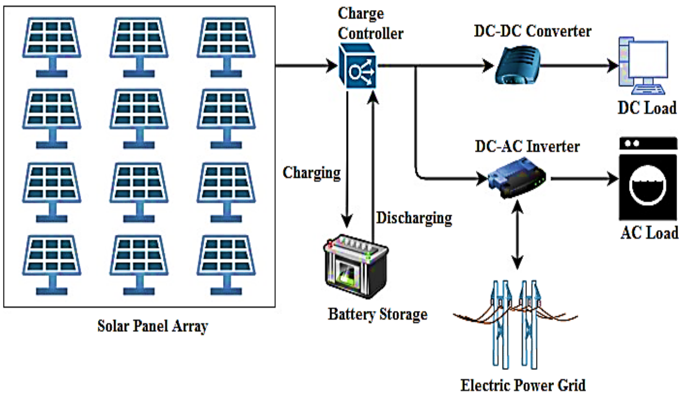

Figure 2. Block diagram showing Rooftop solar panel to grid and domestic appliances

To create a solar array the socket on the other side of the panel are arranged in such a way that their interconnection provide an ease to user through standardized socket. The expansion availability in solar panels make them suitable to accommodate different loads, external circuits, storage batteries and even to grid-systems as shown in Fig. 2

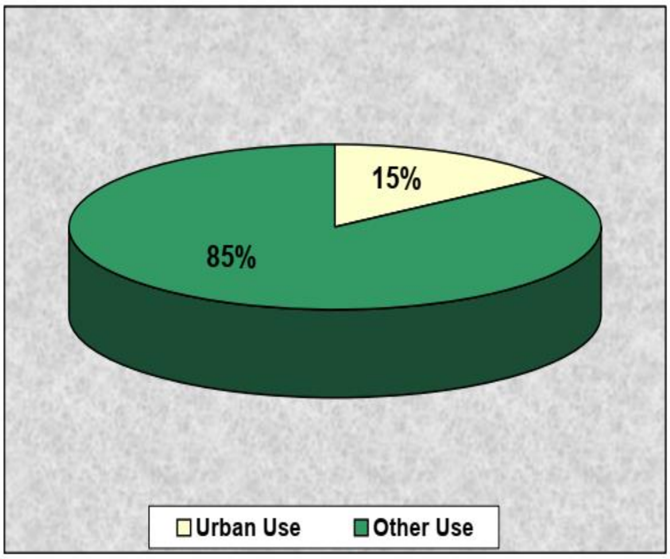

Figure 3. Diagrammatical representation of land use in Shimla city.

A solar system installed for domestic applications is mentioned through its peak power. Like, for proper functioning of equipments in the range upto 1kW, the panel produces 1kW of power per hour on a sunny day. The prime concern is to run domestic appliances on solar energy which require a detailed calculation of how many units of electricity you are consuming on an average in a month. This can be understood using an example:

If you are using 1000 kWh per month, let's assume that an average of 6 hours of solar light per day is available, this shows that you would need 1000/31×6 = 5.38 kW at least every hour which means for efficient functioning on solar energy a 5 – 7 kW system is required. Generally, 7-8 sq. meter of area is required to generate 1kW of solar power.

The following parameters are taken into consideration to examine the size of the plant:

- The average peak load during the summers and in a year
- the load sanctioned
- the available roof area to install panel

The estimated solar irradiation in SHIMLA, is 1046.26 W / sq. 1kWp solar rooftop plant that will generate an average 4.1 kWh of electricity per day (considering 5.5 sunshine hours).

Table 1. Detailed Implementation and Cost Details:

1. Size of Power Plant	**Values**
Feasible Plant size as per Roof Top Area:	10.0Kw
2. Cost of the Plant :	
MNRE current Benchmark Cost :	Rs. 45000 Rs. / Kw
Without subsidy (Based on current MNRE benchmark):	Rs. 450000
With subsidy 40% upto 3kW & 20% above 3kW upto 10kW (Based on current MNRE benchmark):	Rs. 333000
3. Total Electricity Generation from Solar Plant:	
Annual :	**12300kWh**
Life-Time (25 years):	307500kWh
4) Financial Savings :	
a) Tariff @ Rs.5/ kWh (for top slab of traffic) - No increase assumed over 25 years:	
Monthly : **Annually :**	**Rs. 5125** **Rs. 61500**
Life-Time (25 years) :	**Rs. 1537500**
Carbon dioxide emissions mitigated is	**252 tones.**

4. SIMULATION RESULTS AND DISCUSSION

There are various factors that have to be accounted for, in order to represent a real system as a computer model. The consideration of boundary conditions for simulations and description of solar cell unit cell dimensions are illustrated in Table 2 and Table 3. It is extremely difficult to accurately predict the values of some of these factors. Taking appropriate assumptions in the simulation can reduce the complexity while producing fairly accurate results. The assumptions considered for the simulation are:

- All the media are homogeneous and have a uniform refractive index.
- The incident radiations are considered to be unpolarized in nature.
- All material properties are considered isotropic and independent of temperature.
- The top surface of the PV module is assumed to face the mask whereas the back surface is assumed to face the ground. The ground temperature is assumed to be equal to the ambient temperature.

A model can uniquely represent a system when appropriate input and boundary conditions are applied on the model. The boundary conditions that are imposed on the model in this simulation are as follows:

Table 2. Boundary conditions for Multiphysics simulation study of a one-cell module.

S. No.	Parameters	Values
1.	Global Horizontal Irradiance (GHI)	810 W/m²
2.	Direct Normal Irradiance (DNI)	740 W/m²
3.	Mean ambient temperature	32.3 ^{0}C
4.	Mean wind velocity	0.71 m/s
5.	Emissivity of glass	0.85
6.	Emissivity of back surface	0.95
7.	Metal coverage area	0.07% of cell area

The front metallization of the solar cell was not included in the study in order to reduce the complexity of the simulation.

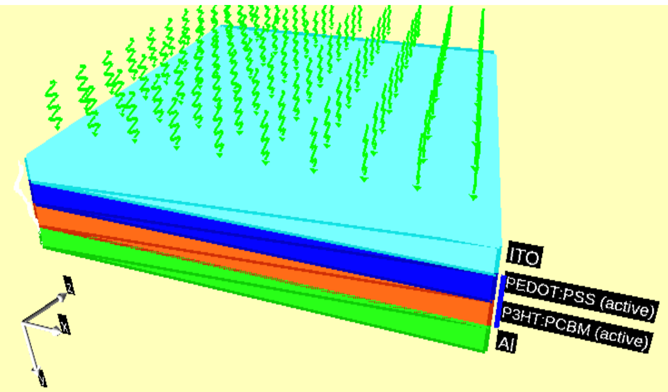

Figure 4. Layer-wise representation of solar cell unit

The device parameters used as input for computer simulation are:

Table 3. Description of layers of Solar Cell unit

S. No.	Layer Name	Thickness (in µm)	Layer Type
1.	Metal Contact (ITO)	0.1	Contact
2.	PEDOT: PSS	0.1	Active Layer
3.	P3HT: PCBM	0.2	Active Layer
4.	Aluminum (Al)	0.1	Contact

The simulation processing data obtained through calculations are mentioned in Table 4. To improve the efficiency of the solar panel the different layers of different polymers are used. The active layer 1 is formed by PEDOT: PSS, or Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate, which is a translucent conductive polymer that consist of mixture of poly(3,4-ethylenedioxythiophene) and polystyrene sulfonate. It has good conductivity, transparent to white light, ductile in nature and easy to process, all these beneficial properties make PEDOT: PSS a useful material in thin film fabrication of solar cells.

Table 4. Simulation Processing Data:

P_{max}	V_{oc} (V)	I_{sc} (mA)	FF	P_{in} (mW/cm²)	Area (cm)²
2.43365	**0.975**	**29.4**	**84.9**	**10.4976**	**3.24**

In organic light emitting diodes it is used as interfacial layer also used in, organic photovoltaics, and perovskite photovoltaics. Its conducing properties make it available to use as transparent conductor in place of ITO or FTO. It is elucidated from Fig. 4 that with the increase in applied voltage across the panel the total charge density start increasing.

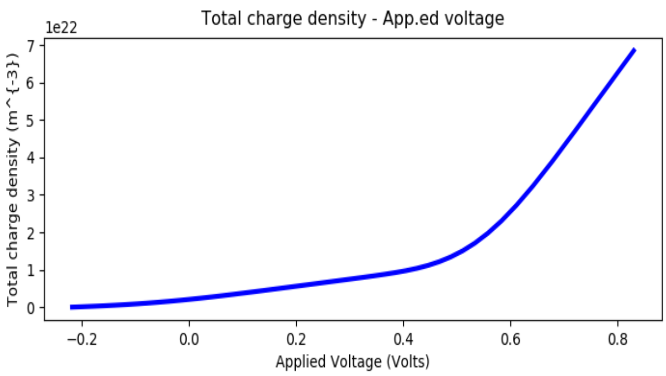

Figure 4. Total Charge Density on application of applied voltage

The second active layer that is used in solar cell unit cell is made of polymer P3HT: PCBM. It is formed by inserting a PCBM (phenyl-C61-butyric acid methyl ester) layer between a P3HT (poly (3-hexythiophene)): PCBM blend.

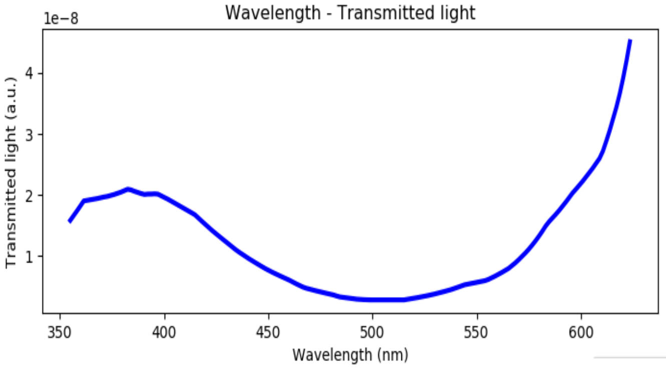

Figure 5. Transmitted light from the surface of the solar panel

This improves the performance of P3HT: PCBM bulk-heterojunction polymer solar cells. By doing so the maximum power conversion efficiency reached 4.24%, which is much higher than that of the traditional standard P3HT: PCBM based device (3.57%). The factor variation of transmitted light with increase in wavelength between visible range can be observed in Fig. 5 which shows that by introducing this layer in combination with PEDOT: PSS it is found that the enhancement of the device performance can be improved. The reason behind these improvements can be defined on the basis of (i) the improvement in atomic structure that gives to improved photocurrent and (ii) suppression of carrier recombination due to increase in PCBM at the layer junction. The electrical properties of the different layers of the proposed solar cell are as follows:

Table 5. Electrical Properties of Active layers of solar cell unit.

S. N.	Electrical Parameters and their units	PEDOT: PSS (Active Layer)	P3HT: PCBM (Active Layer)
1.	Electron trap density ($m^{-3}eV^{-1}$)	8.66e+24	1.52e+27
2.	Hole trap density ($m^{-3}eV^{-1}$)	1.79e+27	7.25e+24
3.	Relative permittivity (au)	3.0	3.8
4.	Effective density of free electron states (@300K) (m^{-3})	5e26	5e16
5.	Effective density of free hole states (@300K) (m^{-3})	5e12	5e26
6.	E_g (eV)	2.1	1.1
7.	Recombination rate constant (m^3s^{-1})	1e-15	1e-7
8.	Free carrier statistics (Type)	Maxwell Boltzmann-analytic	Maxwell Boltzmann-analytic

When a fraction of incident photon flux gets converted into an electric current that phenomenon is termed as external quantum efficiency and spectra related to it is called as external quantum efficiency spectra (EQE) as shown in Fig. 6. It defines the ratio of photons converted to incident. The absorption of all the photons at certain wavelength, positively results into the carrier generation and collection of these carriers by end junctions results to unity value EQE. As absorption of the photons is highly related to absorption coefficient of material and it in turn related to the wavelength of the photon incident on the surface, EQE is also mostly expressed a function of photon wavelength or energy. The simulation model of panel in Comsol Software can be seen in Fig. 7.

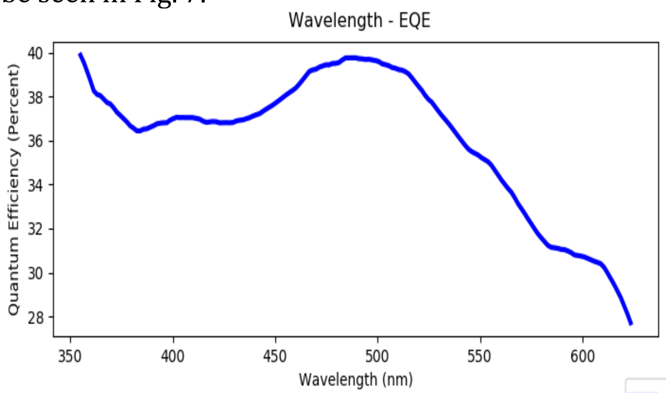

Figure 6. Quantum efficiency versus wavelength

The measurement of EQE curve provides a hint to improve the wavelength. It also depends upon the bias voltages that also affects the collection of photo generated carriers. The Figure 8. shows a comparison of internal quantum efficiency, external quantum efficiency and reflection of the photons from the surface of the solar cell.

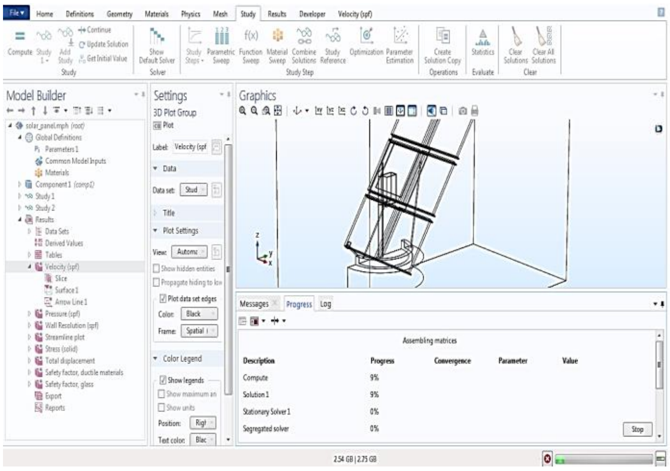

Figure 7. Model under Simulation

Internal quantum efficiency (IQE) measures the probability of contribution of electric charge by an incident photon to the external circuit of the cell. The chance of reflection of photon from the surface of solar panel is more as compared to it absorption. The expectancy of reflection from surface is reduced by applying an anti-reflection (AR) layer. The design of solar panel contains an AR layer that absorb the incident photon and provide near to zero reflectance of the surface at all wavelengths. The internal quantum efficiency is given as ratio of electrons collected as photocurrent per second to the photons absorbed by the surface of the solar panel per second. An ideal material avoids the charge recombination and achieve the value approximately equal to 1. The internal quantum efficiency (IQE) is given as:

$$IQE = \frac{EQE}{1 - Reflection - Transmission} = \frac{electrons / sec}{absorbed photons / sec}$$

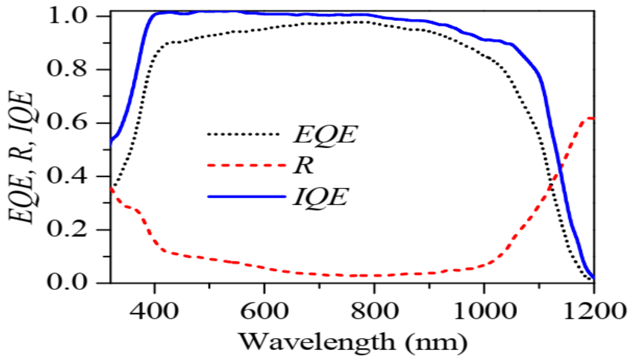

Figure 8. Relative representation of (i) External Quantum Efficiency (EQE), (ii) Internal Quantum Efficiency (IQE), (iii) Reflection of the photons (R) Even neglecting the imperfection and other losses still there is impossible to achieve unity for IQE as parasitic losses and dark current plays a crucial role.

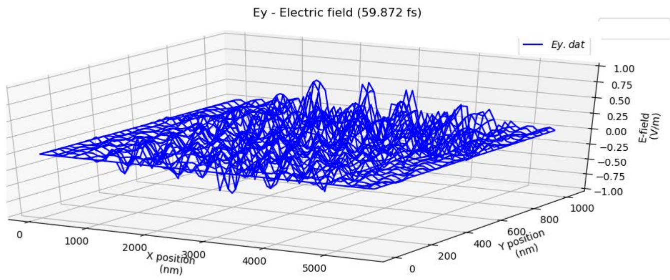

Figure 9. Electric field pattern over the surface of solar cell unit

The electric field pattern over the surface of solar cell unit describes the electrical properties of the solar cell. It results to the widening of junction band which can create more and more free charge carriers can be observed in Fig. 9. Whereas, the planar variation of electric field can be examined using Fig. 10. This shows that field travel over the surface of unit cell results to increase in internal efficiency of the cell.

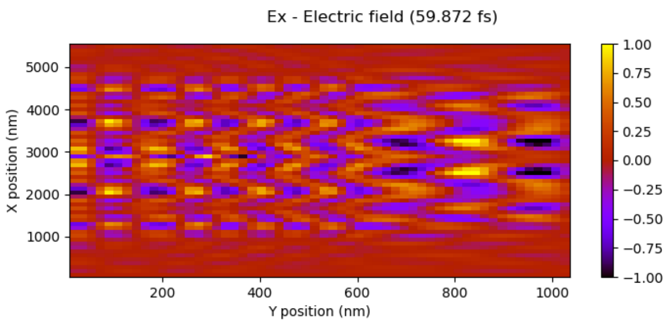

Figure 10. Electric field across the surface of the solar cell

Table 6. Comparison table of different solar cells performance.

S. N.	Cell Type	Area (cm^2)	V_{oc} (V)	J_{sc} (mA/ Cm^2)	FF (%)	Efficiency (%)
1.	Crystalline Si	4.0	0.706	42.2	82.8	24.7
2.	Crystalline GaAs	3.9	1.022	28.2	87.1	25.1
3.	Poly-Si	1.1	0.654	38.1	79.5	19.8
4.	a-Si	1.0	0.887	19.4	74.1	12.7
5.	$CuInGaSe_2$	1.0	0.669	35.7	77.0	18.4
6.	CdTe	1.1	0.848	25.9	74.5	16.4
7.	**PEDOT: PSS and P3HT: PCBM (Proposed)**	**3.24**	**0.975**	**29.4**	**84.9**	**23.8**

Here **Table 6.** describes the different parameters comparison of already existing solar cell with the proposed cell structure. The crystalline Si and GaAs structure are conventional materials used to fabricate the solar panels.

With the addition of polymers and varying the doping concentration the open circuit voltage (V_{oc}), short circuit current (J_{sc}), Form Factor (FF) and efficiency can be improved.

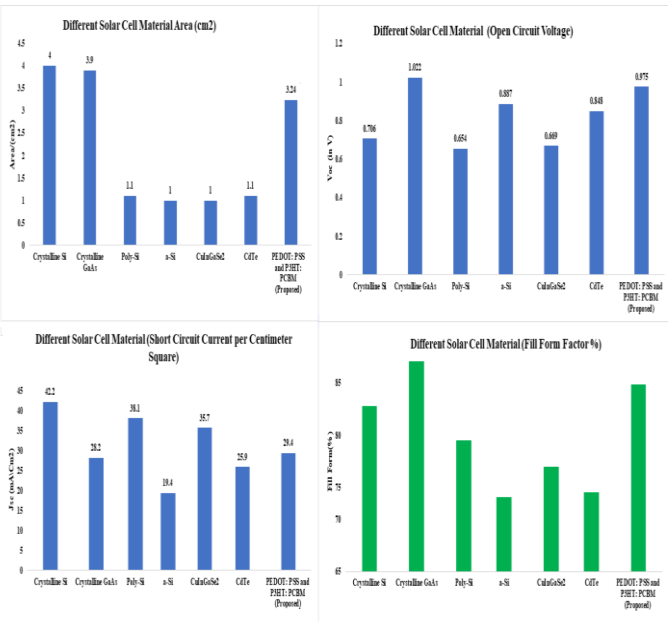

Figure 11. Diagrammatical representation of parameters comparison with the proposed designed solar unit cell.

Through Fig. 11 the values of open circuit voltage, short circuit current and Fill form factor w.r.t to designed area of the unit cells can be examined.

5. CONCLUSIONS

In this paper we presented the principle of operation of solar photovoltaic cell, design and working of hetero structure layer solar cell and its fabrication process. The proposed structure of solar cell is composed of PEDOT: PSS and P3HT: PCBM working as active layer and create a junction that results to free charge carriers upon illumination to solar light. These two polymers are considered for the fabrication and simulation of the solar cell because these are 4th generation materials used for fabrication of solar cell. The efficiency of the solar cell depends upon the wavelength and at atomic level to the doping concentration. The energy band gap of the polymers is low as compared to the other conventional materials so the generation of charged carriers are more as compared to other and also the recombination rate is low due to conductivity and thickness. The dimensions and parameters are mentioned above leads to various results and improved overall efficiency of 23.8% which can improve the short circuit current and open circuit voltage. The 3rd and 4th generation solar cells can be looked as substitute for non-renewable energy sources. This will not only satisfy the demand of power consumption but also create a clean and green environment.

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