# SYNTHESIS CHARACTERIZATION AND THEORETICAL MODELING OF SOLAR CELL AND MATERIALS

M.Sc. Thesis

By SHOBHIT KUSHWAHA



## DISCIPLINE OF PHYSICS INDIAN INSTITUTE OF TECHNOLOGY INDORE MAY 2024

# SYNTHESIS CHARACTERIZATION AND THEORETICAL MODELING OF SOLAR CELL AND MATERIALS

### **A THESIS**

Submitted in partial fulfilment of the requirements for the award of the degree of Master of Science

> *by* **SHOBHIT KUSHWAHA**



## DISCIPLINE OF PHYSICS INDIAN INSTITUTE OF TECHNOLOGY INDORE MAY 2024



## **INDIAN INSTITUTE OF TECHNOLOGY INDORE**

### **CANDIDATE'S DECLARATION**

I hereby certify that the work being presented in the thesis entitled "Synthesis Characterization and Theoretical Modeling of Solar Cell and Materials" in the partial fulfillment of the requirements for the award of the degree of MASTER OF SCIENCE and submitted in the DISCIPLINE OF PHYSICS, Indian Institute of Technology Indore, is an authentic record of my work carried out during the time period from August 2022 to May 2024 under the supervision of Prof. Pankaj R. Sagdeo department of physics IIT Indore.

The matter presented in this thesis has not been submitted by me for the award of any other degree of this or any other institute.

Shabhit Kushwaha) 24 | 05 | 2024

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This is to certify that the above statement made by the candidate is correct to the best of my/our knowledge.

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Shobhit Kushwaha Master of Science Department of physics Indian Institute of Technology Indore

Dedicated to

My parents

And teachers

#### Abstract

The present work focuses on one of the most important external parameter of the solar cell the opencircuit voltage( $V_{oc}$ ), It is confirmed by performing simulations on various single junction photovoltaic technologies such as homojunction solar cells based on GaAs and Ge absorber material, heterojunction solar cells based on CdTe absorber material, perovskite solar cells based on CsGeI<sub>3</sub> absorber material, that the open-circuit voltage( $V_{oc}$ ) is determined by the extent to which the quasi-fermi level  $E_{Fn}$ and  $E_{Fp}$  are able to split. The splitting of the quasi-fermi level is limited by the recombination mechanism due to the presence of the defect in the solar cell, which leads to a deficit in open-circuit voltage which is reflected in terms of the Urbach energy ( $E_U$ ), However, the exact explicit quantitative analysis is not available yet so by using numerical simulation methodology on thin-film CdTe photovoltaic (PV) solar cell we picturize the effect of the Urbach energy ( $E_U$ ) in the open-circuit voltage( $V_{oc}$ ), and observe the power conversion efficiency (PCE) of the solar cell. which makes the strong argument that Urbach energy ( $E_U$ ) become an important diagnostic parameter to study the loss mechanism associated with the solar cell.

In addition to investigating the loss mechanism, there has been an exploration into the generation mechanism of the single junction solar cell as well. This exploration falls under the section of device optimization, a simulation-based optimization technique proves highly effective, significantly reducing both time and labor-intensive tasks, the optimization procedure begins by optimizing the thickness of the ETL (Electron Transport Layer), HTL (Hole Transport Layer), and absorber layer. Surprisingly, the thickness of the HTL does not impact device performance. However, the thickness of the ETL and absorber material significantly affects performance. Finally, optimization of the absorber acceptor concentration is conducted. Initially, an unoptimized device have an efficiency of 16.47%. After optimization, the efficiency increases to 22.49%. As far as single-junction solar cells are concerned, even the extremely fine-tuned(optimized) device has a limit of maximum attainable efficiency, limited spectral utilization by the single-junction solar cell restricts the maximum theoretical conversion limit well known as the Shockley Quieeser limit, this can be overcome by exploiting the much part of the solar spectrum using multiple junctions. Simulating multijunction solar cells with the SCAPS-1D tool is more complex rather than simulating single-junction cells. The process involves simulating individual subcells, and then connecting them in series using SCAPS-1D script support. This procedure is more time-consuming compared to single-junction cell simulation. A task of simulating a two-junction solar cell has been performed, In the first step top cell GaAs ( a higher band

gap material) is designed individually and a complete AM 1.5 spectrum is made to incident on it, the second step involves designing the bottom cell Ge(a low band gap material) a filtered AM 1.5 spectrum(solar radiation that is not utilized by the top cell) is made to incident on it, finally using Scaps-1D script support connect them in the series and extract the external parameters of the two -junction solar cell, the resultant efficiency of the simulated two-junction solar cell comes out to be 28.10%, which is far higher than the efficiency produces by the individual top cell(23%) and individual bottom cell(7.36%) at standard test condition.

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## Abbreviations

J <sub>PH</sub>	Photo-generated current density			
J <sub>Dark</sub>	Diode current at dark			
Jo	Reverse saturation current density			
V <sub>OC</sub>	Open-circuit voltage			
Jsc	Short circuit current density			
FF	Fill factor			
PEC	Power conversion efficiency			
QE	Quantum efficiency			
R <sub>sh</sub>	Shunt resistance			
$R_S$	Series resistance			
$E_U$	Urbach Energy			
eta	Power conversion efficiency			
ETL	Electron transport layer			
HTL	Hole transport layer			
FTO	Fluorine doped tin oxide			

### Chapter 1 -Fundamentals of Solar Cell

#### **1.1 Introduction**

The solar cell is a photovoltaic device whose electrical response (conductivity, resistivity, etc.) varies with the radiation exposure, Which is employed to harness energy from the sun spectrum, present as an abundant source of energy. Starting with the solar cell working and its characteristics J-V curve, equivalent circuit, external parameters which are used to characterize the performance of different technology-based solar cells and differentiating between practical and ideal solar cells will be enveloped in this chapter with a simulation-guided approach using simulator tool SCAPS-1D. A brief description of the simulator will be provided in chapter2.

#### 1.2 Working and J-V characteristics of Solar cell

The functionality of a solar cell can be divided into three basic attributes as follows

- Optical excitation results in the production of electron-hole pair and/or Exciton[1](an electronic entity which is the bound state of electron and hole due to columbic interaction).
- These optically generated entities are separated with the help of an internal built-in electric field.
- And the extraction of those charge carriers to the back and the front contact.

Solar cell device performance is governed by the external parameters which can be extracted by making use of characteristics J-V curve. For illustration purposes, a GaAs-based solar cell structure has been simulated(For detailed information, please refer to Section 2.4) in the dark as well as in an illuminated condition reflected by red and blue curves respectively Figure1.1. The downward shift in an illuminated J-V curve with respect to dark can be understood by making an argument that illumination results significant increase in minority charge carriers leading to large drift current, overall diode current density is given by the equation.1[1].

$$J = J_{PH} - J_{Dark}$$
$$J = J_{PH} - J_0 \left( \exp\left(\frac{qV}{k_BT}\right) - 1 \right) \qquad \dots 1$$

Where  $J_{PH}$  stand for the photo-generated current density and  $J_0$  is the reverse saturation current density in the dark, all notations have usual meaning and can be found elsewhere.



Figure 1.1 Simulated J-V curve of the GaAs solar cell in dark and illuminated condition reflected by red and blue curves respectively

#### 1.3 Equivalent circuit of ideal Solar cell

The equivalent circuit of a solar cell is a theoretical representation that is employed to study the electrical behavior of a solar cell, in the upcoming section, this model can also be exploited to characterize the solar cell, that deviated from ideality[2].



Figure 1.2 Equivalent Circuit

From Figure 1.2 one can observe that  $I_D$  is dark current, due to diffusion of charge carrier in forward bias, and when the junction is illuminated due to a significant increase in minority charge carrier a large drift current is established which is opposite to the dark current which is indicated as  $I_{PH}$  (photo generated current).

#### 1.4 External parameters of ideal Solar cell

These are the parameters that are used to compare the performance of different technologies of solar cells and how efficiently they convert light energy into electrical energy.

#### 1.4.1 Open-circuit voltage

Electrical properties of semiconductors are governed by charge carrier concentration in the material which obeys Fermi-Dirac distribution[3]. In dark equilibrium condition (with no bias) there is only a single Fermi level ( $E_F$ ) Throughout the device which gives the significance of electron-hole concentration throughout the device, when the equilibrium is disturbed on exposure to radiation, and allowed to reach quasi-equilibrium, obviously now concentration will no longer be the same as earlier, to state electron and hole concentration throughout the device two separate fermi level  $E_{Fn}$  and  $E_{Fp}$  were taken which are termed a quasi-fermi level[3].



Figure 1.3 Energy versus position band diagram of GaAs solar cell (a) in dark and (b)illuminated condition

For illustration purposes again simulation on GaAs based solar cell has been performed in Figure 1.3(a) energy band diagram of a GaAs-based solar cell in the dark at equilibrium, one can see that there is only a single fermi level which is reflected by the red colour straight line, on the other hand in Figure 1.3(b) energy band diagram of the same cell at illuminated condition, there are two fermi level  $E_{Fn}$  and  $E_{Fp}$  reflected by blue and red colour respectively.

The open-circuit voltage ( $V_{oc}$ ) is determined by the extent to which quasi fermi level is able to split, which is further limited by the recombination mechanisms associated within the solar cell[4]. The higher the splitting in the quasi-fermi level higher will be the open-circuit voltage.



Figure 1.4 (a) High splitting in quasi fermi level when defect concentration is low (b)Less splitting in quasi fermi level when defect concentration is high



Figure 1.5 (i) J-V curve when splitting is low (ii) J-V concentration when splitting is high

Simulation has been performed again on a GaAs-based solar cell structure. Figure1.4(a) energy band diagram when defect concentration is low, results in less recombination of optically generated charge carriers as a consequence higher splitting in quasi fermi-level, Figure1.4(b) reflects the energy band diagram when defect concentration is high, which results in high recombination of optically generated charge carriers as a consequence lesser splitting in quasi-fermi level.

Figure 1.5 (i) J-V curve when defect concentration is high and (ii) when defect concentration is low, comparatively open-circuit voltage (in the open circuit the solar cell does not produce any current i.e. current density is zero) is high when defect concentration is low, which leads to less recombination and

higher splitting in quasi fermi level. The mathematical form of open-circuit voltage can be derived from equation 1.1.

$$J = J_{PH} - J_0 \left( \exp\left(\frac{qV}{k_B T}\right) - 1 \right) \qquad \dots 1.1$$

Putting J = 0 and  $V = V_{OC}$  because in open-circuit voltage solar cells do not produce any current. The above expression can be reduced to

$$V_{OC} = \frac{k_B T}{q} \ln \left( \frac{J_{PH}}{J_0} + 1 \right) \qquad \dots 1.2$$

Factors on which  $V_{OC}$  depends

- Depend on photocurrent density  $(J_{PH})$  i.e. by increasing the irradiance or shining more and more light on the solar cell, the  $V_{OC}$  can be increased.
- Higher the temperature the larger the leakage current density  $(J_0)$  and smaller the  $V_{OC}$ .

#### **1.4.2** Short circuit current density( $J_{SC}$ )

It is the current density generated by the solar cell under a short circuit (voltage across the output terminal should be zero) condition.

The mathematical expression of the  $J_{SC}$  can be obtained by using equation 1.1.

$$J = J_{PH} - J_0 \left( \exp\left(\frac{qV}{k_B T}\right) - 1 \right)$$

Putting V = 0 and  $J = J_{SC}$  we get;

$$J_{SC} = J_{PH}$$

Hence,  $J_{SC}$  is equivalent to  $J_{PH}$  (photo-generated current density).

#### 1.4.3 Power density

The term power density is defined as the product of current density and voltage, the green colour curve in Figure 1.6 corresponds to the power density curve and the red colour curve corresponds to the J-V curve of the solar cell. using the power density curve, we can find the maximum operating power point further which can used to calculate the FF and the PCE of the solar cell.



Figure 1.6 J-V and power density curve

Some important arguments can be made regarding the power density curve as follows: -

- When the power density is negative, it indicates that the solar cell is producing power.
- When the power density is positive, it indicates that the solar cell is dissipation power.
- On the J-V curve shown where power density is maximum called maximum power point  $(P_{max})$ .
- Where voltage is smaller than zero, which is reverse bias, the illuminated solar cell does not generate power but consumes power.
- Also, when if voltage of the solar cell is greater than the  $V_{OC}$  the illuminated solar cell dissipates power as well.
- The solar cell will have the best performance at its maximum power point at

$$V = V_{MPP}$$
 and  $J = J_{MPP}$ 

This means

$$P_{max} = V_{MPP} J_{MPP} \qquad \dots 1.3$$

#### **1.4.4** Fill Factor(FF)

The term fill factor can be defined as the ratio of, the ratio of the product of the maximum operating point to the product of  $J_{SC}$  and  $V_{OC}$ .

$$FF = \frac{P_{max}}{J_{SC}V_{OC}} = \frac{J_{MPP} V_{MPP}}{J_{SC}V_{OC}} \qquad \dots 1.4$$

#### It implies that it is impossible for a solar cell to have a FF equal to 1.

Another empirical relation of the FF proposed by Martin A. Green, when the diode ideality factor(n)[5] is known under the assumption of series resistance to be zero and shunt resistance to be infinite [6].

$$FF = \frac{v_{oc} - \ln(v_{oc} + 0.72)}{v_{oc} + 1} \qquad \dots 1.5$$

Where,

$$v_{oc} = \frac{qV_{OC}}{nk_BT}$$

#### **1.4.5** Power Conversion Efficiency(PEC)

This is the ratio of  $P_{max}$ (maximum power density coming out of the solar cell) and the  $P_{in}$ (light power density) of light incident on the solar cell.

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_{MPP}J_{MPP}}{P_{in}} \qquad \dots 1.6$$

#### **1.4.6** Quantum efficiency(QE)

The term Quantum efficiency is used to measure the Spectral utilization of solar cells, it gives the significance of which part of the solar spectrum is utilized efficiently, (the detailed analysis is provided in section 4.2).

The QE( $\lambda$ ) is the ratio of the number of carriers collected at the terminals per incoming photon at a certain wavelength[7]. QE is the function of wavelength

The mathematical expression is given by.

$$QE(\lambda) = \frac{J_{sc}/q}{\varphi(\lambda)} \qquad \dots 1.7$$

Where,

 $\varphi(\lambda)$  is photon flux at a certain wavelength.

If all the photons participated in charge collection, then QE=1.

The reduced quantum efficiency is attributed to various electrical and optical loss mechanisms.

Photons can be reflected back from the front entrance of the cell, the Figure 1.7(a) below illustrates the effect of reflection in QE.

- Photons do not absorb as they have energy less than the band gap.
- > The absorber layer is excessively thin.
- The recombination of light-excited charge carriers, Figure 1.7 (b) below illustrates the effect of recombination in QE when defect density is increased resulting in the recombination of charge carrier.



Figure 1.7 Variation of QE with (a) reflection of photons and (b) increasing defect density

From equation 1.7 one can also find the maximum limiting value of the  $J_{SC}$  (short circuit current density) of the various technologies of solar based on its spectral response[8].

$$J_{SC} = q \int_{0}^{\lambda} \varphi_{A.M \, 1.5}(\lambda) \, EQE(\lambda) \, d\lambda \qquad \dots 1.8$$

#### 1.5 Practical or non-ideal Solar cell

Solar cells consist of several layers of semiconductor, back contact, and front contact, and the interface forming between contact and semiconductor has inherent resistance which is responsible for the series resistance in solar cells represented by  $R_S$  [9], while processing cells some manufacturing defects that are capable of providing alternative paths to flow photogenerated current within the solar is responsible for shunt resistance denoted by  $R_{SH}$ . A good-quality cell must have a high  $R_{SH}$  (shunt resistance) and low  $R_S$  (series resistance). To analyze the effect of  $R_S$  and  $R_{SH}$  again simulation has been performed on GaAs-based solar cell.

#### **1.5.1** Series Resistance( $R_S$ )

Performing simulation on GaAs-based solar cell,  $R_S$  varied from 0 ohm cm<sup>-2</sup> to 10 ohm cm<sup>-2</sup>, the influence of series resistance on open-circuit voltage( $V_{OC}$ ) is very little but has a significant impact on  $J_{SC}$ (short-circuit current density), which leads to a decrease in device performance.

According to simulated data on varying series resistance form (0-10) ohm cm<sup>-2</sup> short circuit current density reduced from 25.9134 mAcm<sup>-2</sup> to 25.9082 mAcm<sup>-2</sup> which leads to a significant decrease in FF from 87.78% to 64.46% and PCE reduced from 23.24% to 17.07%. The variation of PCE and FF with respect to series resistance has been plotted in Figure 1.8 (a) and Figure 1.8 (b) respectively.



Figure 1.8 Impact on J-V curve with series resistance



Figure 1.9 Impact of series resistance on (a) PCE and (b) FF

#### **1.5.2** Shunt Resistance( $R_{SH}$ )

Performing simulation on GaAs-based solar cell, shunt resistance varies from 1000 ohm cm<sup>-2</sup> to 100 ohm cm<sup>-2</sup>, the influence of shunt resistance on short circuit current density ( $J_{SC}$ ) is very less but has a significant impact on open-circuit voltage ( $V_{OC}$ ), which leads to degradation in the performance of the device.

According to simulated data on varying shunt resistance from (1000-100) ohm cm<sup>-2</sup>  $V_{OC}$  (open-circuit voltage) reduced from 1.02 volt to 1.00 volt which led to a significant decrease in fill factor from 84.66% to 56.98% and PCE reduced from 22.39% to 14.93%. The variation of PCE and FF concerning series resistance has been plotted in Figure 1.11(a) and Figure 1.11(b) respectively.



Figure 1.10 Impact on J-V curve with shunt resistance



Figure 1.11 Impact of shunt resistance on (a) PCE and (b) FF

### 1.6 Summary

This chapter covers the operation of solar cells and explains how the current-voltage (J-V) curve shifts downward under illumination compared to dark conditions due to the dominance of the large drift current. To compare the performance of different solar cell technologies, we use external parameters. For non-ideal solar cells, their behaviour can be studied by adding series and shunt resistance to the equivalent circuit.

### Chapter 2 <u>-Simulation of various photovoltaic technology based</u> on single junction solar cell using Scaps-1D

#### 2.1 Introduction to Scaps-1D Simulator Tool

Solar cell research has made significant advancements in recent years, but it still faces several challenges and problems that researchers are actively working to address. Some of the key problems are[10].

I)- Efficiency Improvement	IV)- Environmental Impact		
II)- Cost Reduction	V)- Scalability		
III)- Energy Storage	VI)- Durability and reliability		

etc. some other factors like Government policies, incentives, and regulations can significantly impact the solar industry.[11].

Researchers in the field of solar cells are actively working on these challenges to make solar energy more accessible, efficient, and sustainable. Collaboration between scientists, engineers, policymakers, and industry stakeholders is vital to overcoming these obstacles and advancing the adoption of solar energy worldwide. In order to overcome these challenges without doing much laborious work or we can hand over our work to machine(computer). There is a requirement for some simulation software, which can help us to give our work to the computer.

Solar cell simulation can significantly reduce research and development costs as well as time. Instead of building and testing multiple physical prototypes, researchers can use simulation to explore various design options and parameter settings at a fraction of the cost and time. In this wonderful journey of research and development, there is one most widely and commonly used simulation tool "SCAPS-1D".

SCAPS-1D is a well-known simulator tool widely for the simulation of CdTe-based photovoltaic cell[12], [13] and perovskite photovoltaic cells[14], which was refined at the University of Gent, Belgium. SCAPS (Solar Cell Capacitance Simulation in 1D) is a specialized software tool designed for simulating and analyzing the electrical characteristics of semiconductor solar cells, particularly photovoltaic (PV) devices. SCAPS-1D focuses on one-dimensional simulations, effectively modeling the behaviour of solar cells based on their depth profile within the device structure.

This is a thorough description of the tool, which is thought to be useful for photovoltaic research, numerical design, and modeling of solar cells. Tools like SCAPS-1D give a mathematical overview of the drift and diffusion model, enabling one to comprehend how devices work and forecast their physical behaviour. Without requiring significant financial, human, or time commitments, this computational tool facilitates the exploration of several critical parameters, thickness, electron affinity, carrier concentration, band gap, defects density, surface recombination velocity, shunt and series resistances, work function, and temperature. Essentially, SCAPS-1D is a collection of several fundamental equations, which are represented as follows: the Poisson equation, the electron continuity and hole continuity equations, and the hole and electron current density equation.[1], [3], [15], [16].

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{q}{\varepsilon} \left[ p(x) - n(x) + N_D - N_A + \rho_p - \rho_n \right] = 0 \qquad \dots 2.1$$

$$\frac{1}{q}\frac{dJ_p}{dx} = G_{op}(x) - R(x) \qquad ...2.2$$

$$\frac{1}{q}\frac{dJ_n}{dx} = -G_{op}(x) + R(x) \qquad ... 2.3$$

$$J_n = qn\mu_n E + qD_n \frac{\partial n}{\partial x} \qquad \dots 2.4$$

$$J_p = qn\mu_p E - qD_p \frac{\partial p}{\partial x} \qquad \dots 2.5$$

where  $N_D$  and  $N_A$  represent the donor and acceptor concentration;  $J_p$  and  $J_n$  stands for the current density of the hole and electron; n and p represent the electron and hole concentration in conduction and valence band respectively and  $\rho_n$  and  $\rho_p$  are the trapped electron and trapped hole concentrations, respectively. R indicates the total losses from direct and indirect recombination; however, Gop signifies the optical generation rate;  $\Psi$  is the electrostatic potential [17].

#### 2.2 Simulation of lead-free CsGeI3-based perovskite Solar cell

Perovskite solar cell based on organic-inorganic halides such as  $MAPbI_3$  and  $FAPbI_3$  has a record efficiency of above 23%[18], but the major obstacle in large-scale commercialization is the presence of harmful toxic element lead[19]. With this motivation, there is a requirement for alternate lead-free perovskite solar cells.

#### 2.2.1 Device Structure

The Figure 2.1(a) below illustrates the device structure based on  $CsGeI_3[20]$  and a screenshot of the window panel of Scaps-1D in Figure 2.1(b) reflects the different layers of the solar cell.



Figure 2.1 (a) Cell structure (b) Screenshot of the simulator pannel confuguring the same structure

In the above cell solar radiation enters from the front layer FTO and on top of that  $TiO_2$  layer is deposited, due to the presence of  $TiO_2$  percolating network the generated electron can be rapidly transferred to the FTO, above it absorber layer CsGeI<sub>3</sub> were deposited, on top of it a hole transport layer(HTL) Spiro-OMeTAD is deposited which rapidly collect hole and transferred to back contact of the solar cell(Ag) work function of back contact is taken to be 4.46eV.

#### 2.2.2 Methodology for Scaps-1D simulation

Simulation of the devices required various input parameters that are gathered from diverse theoretical and experimental investigations and are arranged in Table2-1[16], [17], [20], [21], [22], [23].

Parameters	Spiro- OMeTAD	CsGeI <sub>3</sub>	TiO <sub>2</sub>	FTO
Thickness(nm)	200	400	30	500
Bandgap(eV)	2.88	1.6	3.2	3.2
Dielectric Constant	3.00	18	9	9
Electron affinity(eV)	2.050	3.520	3.9	4.00
$N_C(1/\mathrm{cm}^3)$	2.200E+18	1.00E+18	2.200E+18	2.200E+18
$N_V(1/\mathrm{cm}^3)$	1.800E+19	1.00E+19	1.00E+19	1.800E+19
$V_e(\text{cm/s})$	1.00E+7	1.00E+7	1.00E+7	1.00E+7
$V_h$ (cm/s)	1.00E+7	1.00E+7	1.00E+7	1.00E+7
$\mu_e(\mathrm{cm}^2/\mathrm{Vs})$	2.100E-3	2.00E+1	2.00E+1	2.00E+1
$\mu_h \ (\mathrm{cm}^2/\mathrm{Vs})$	2.600E-3	2.00E+1	1.00E+1	1.00E+1
$N_D(1/cm^3)$	0.00E+0	0.00E+0	1.00E+18	1.00E+19
$N_A(1/cm^3)$	2.00E+19	2.00E+16	0.00E+0	0.00E+0
$\tau_e(\mathrm{ns})$	100	100	5	1000
$\tau_h(\mathrm{ns})$	100	100	5	1000
Neutral defect density(1/cm <sup>3</sup> )	1.00E+15	1.00E+15	1.00E+15	1.00E+14

Table 2-1 Electrical parameters corresponding to different layers regarding simulation of CsGel3 solar cell

The notations that are used above can be easily found elsewhere.

Here we are dealing with a thin film technology involving various layers with the thickness of the order of nanometre(nm), apart from the bulk recombination surface recombination becomes dominant, so the interface forming between two layers becomes a channel for the recombination of optically generated charge carriers [24]. The screenshot of the introduced defect between the interface forming between absorber material and electron transport material (CsGeI<sub>3</sub>/TiO<sub>2</sub> interface) and absorber material and hole transport layer(Spiro-OMeTAD/CsGeI<sub>3</sub>interface) are depicted in Figure2.2(a) and Figure2.2(b) respectively.

SCAPS 3.3.10 Interface Defect Properties Pane	el — 🗆	$\times$	SCAPS 3.3.10 Interface Defect Properties Panel	- 0 X
Defect 1 of CsGel3 / TiO2 interface			Defect 1 of Spiro-OMeTAD / CsGel3 interface	
defect type	neutral	-	defect type	neutral -
capture cross section electrons (cm²)	1.00E-15		capture cross section electrons (cm <sup>2</sup> )	1.00E-15
capture cross section holes (cm²)	1.00E-15		capture cross section holes (cm2)	1.00E-19
energetic distribution	single	-	energetic distribution	single 👻
reference for defect energy level Et	above the highest EV	-	reference for defect energy level Et	above the highest EV 🗢
energy with respect to Reference (eV)	0.600		energy with respect to Reference (eV)	0.600
characteristic energy (eV)	0.100		characteristic energy (eV)	0.100
total density (integrated over all energies) (1/cm <sup>2</sup> )	1.00E+16		total density (integrated over all energies) (1/cm^2)	1.00E+16
Allow tunneling to interface traps			Allow tunneling to interface traps	
Relative mass of electrons	1.000E+0		Relative mass of electrons	1.000E+0
Relative mass of holes 1.000E+0			Relative mass of holes 1.000E+0	
acceptcance			accept	
(a	)		(b)	

Figure 2.2 Screenshot of the simulator panel representing the defect between the interface (a)CsGel<sub>3</sub>/Tio<sub>2</sub> and (b)  $HTL/CsGel_3$ 

#### 2.2.3 Result of simulation of CsGeI<sub>3</sub>

Initially, energy versus position band diagrams were simulated under both dark and illuminated conditions and are depicted in Figure 2.3(a) and Figure 2.3(b), respectively. In the dark, no external bias is applied, and there is only a single Fermi level throughout the device, which gives the concentration of electrons and holes, represented by the red straight line, after exposure to radiation charge concentration will no longer remain the same; a fermi level has been split into two quasi fermi levels,  $E_{Fn}$  and  $E_{Fp}$  which signifies the concentration of electrons and holes throughout the device, respectively.



Figure 2.3 Energy versus position band diagram at (a) dark equilibrium (b) illuminated condition

With the help of the energy versus position band diagram, we can also explain the movement and collection of charge carriers(electrons and holes). As soon as the device is exposed to the radiation the generation of electron and hole pair will take place(specifically focusing on the absorber material CsGeI<sub>3</sub>), those generated charge carriers will diffuse randomly, and the electron which diffuses towards

ETL will easily collect at the front contact FTO because there is no potential barrier, but the electrons which diffuse towards HTL layer will encounter high potential barrier so, reflected back and get collected at FTO which is the front contact. Similarly, the holes that diffuse towards HTL will easily get collected at back contact because there is no potential barrier on the other hand the holes that diffuse towards ETL will encounter a high energy barrier, so they will be reflected back and get collected at the back contact.

External parameters and QE of the above simulated solar cell have been extracted and are summarized in Table2-2 along with the comparison of experimental work.

External Parameters	V <sub>oc</sub> (volt)	$J_{SC}(mA/cm^2)$	<b>FF</b> (%)	<b>PCE</b> (%)
Experimental[20]	0.51	18.78	51	4.94
Simulated	0.5050	17.89	54.76	4.95

Table 2-2 Comparing the experimental and simulated work on CsGeI3 solar cells



Figure 2.4 comparison of the experimental and simulated work (a) J-V curve and (b) QE curve

The rollover effect in the simulated J-V curve is due to the opposite bias of the back contact in comparison to the solar cell, this effect can be explained by using two diode model[25], in addition, one can use flat band condition instead of using the working function for the back contact which results in no rollover of J-V curve. Deviation in the Quantum efficiency curve is while simulating we didn't consider any reflection and transmission(optical losses) that is why QE is higher in simulated work.

#### 2.3 Simulation of CdTe heterostructure Solar cell

The Simulated structure of a CdTe solar cell is represented in Figure 2.5(a)[26] and Figure 2.5(b).

Again, the device parameters corresponding to various layers were collected from several research papers, and the following has been arranged in Table2-3[26], [27], [28], [29], [30], [31].


(a)

Figure 2.5 (a) Cell structure (b) Screenshot of the simulator panel configuring the same CdTe structure

Parameters	CdTe	CdS	SnO <sub>2</sub>	FTO
Thickness(µm)	6.00	0.10	0.10	0.400
Bandgap(eV)	1.5	2.42	3.6	3.6
Dielectric constant	9.40	10.00	9.00	9.00
Electron affinity(eV)	4.28	4.30	4.50	4.50
$N_c(1/\mathrm{cm}^3)$	8.00E+17	2.20E+18	2.200E+18	2.200E+18
$N_V(1/\mathrm{cm}^3)$	1.800E+19	1.80E+19	1.80E+19	1.800E+19
$V_e(\mathrm{cm/s})$	1.00E+7	1.00E+7	1.00E+7	1.00E+7
$V_h(\text{cm/s})$	1.00E+7	1.00E+7	1.00E+7	1.00E+7
$\mu_e(\mathrm{cm}^2/\mathrm{Vs})$	3.200E+2	1.00E+2	1.00E+2	1.00E+2
$\mu_h(\mathrm{cm}^2/\mathrm{Vs})$	6.00E+1	2.50E+1	2.50E+1	2.50E+1
$N_D(1/cm^3)$	0.00E+0	1.10E+18	1.00E+18	1.00E+19
$N_A(1/cm^3)$	2.00E+14	0.00E+00	0.00E+0	0.00E+0
$\tau_e(\mathrm{ns})$	1	0.1	100	100
$ au_h(\mathrm{ns})$	1	1	0.1	0.1
Neutral defect density(1/cm <sup>3</sup> )	1.00E+15	1.00E+15	1.00E+15	1.00E+15

Table 2-3 Electrical parameters corresponding to different layers regarding simulation of CdTe solar cell

#### 2.3.1 **Result of simulation of CdTe heterostructure solar cell**



Figure 2.6 Energy versus position band diagram of the CdTe cell at (a) dark and (b) illuminated condition

Figure 2.6(a) and Figure 2.6(b) represent the energy versus position band diagram in dark illuminated equilibrium conditions respectively, the movement and collection of the charge carrier process is similar to the above explained in section 2.2.3.

The external parameters and QE of the simulated solar cell mentioned above have been extracted and are presented in Table 2-4, alongside a comparative analysis of experimental findings.

Table 2-4 Comparing the experimental and the simulated work on CdTe solar cells

External Parameters	V <sub>oc</sub> (volt)	$J_{SC}(mA/cm^2)$	<b>FF</b> (%)	<b>PCE</b> (%)
Experimental[26]	0.82	25.60	66.40	14
Simulated	0.81	23.95	69.98	13.64



(a)

Figure 2.7 comparison of the experimental and the simulated work (a) J-V curve and (b) QE curve

Figure 2.7(a) and Figure 2.17(b) correspond to the J-V curve and the QE curve of the simulated CdTe solar cell Fill factor of the simulated cell is much greater in magnitude as compared to the experimental one which can be further reduced by adding some series and shunt resistance, the divergence in QE below 850nm wavelength is due no reflection considered from the front surface, deviation after 850nm to 900nm is due to that in real sample electronic defect in semiconductor leads to the formation of Urbach tails near the valence and the conduction band which results in shifting the absorption towards higher wavelength region.

## 2.4 Simulation of GaAs-based Solar Cell

The structure that has been opted for the simulation is taken from the reference[32], a schematic diagram is depicted in Figure 2.8. Losses associated with the solar cell are such as radiative recombination, the radiative recombination coefficient of  $1.00E-10(\text{cm}^3/\text{s})$  introduced in the emitter, base, BSF layer, and of  $1.20E-10(\text{cm}^3/\text{s})$  introduced at the window layer, neutral defect at 0.71eV above valance band has been introduced with a defect density of  $5.00E+14 \text{ cm}^{-3}$  and  $5.00E+13 \text{ cm}^{-3}$  in the emitter and base layer respectively.



Figure 2.8 GaAs simulated solar cell structure

According to the simulation methodology using SCAPS-1D there are various required parameters that can be extracted from various literature surveys and are tabulated in the table5[32], [33], [34], [35].

Parameters	Al <sub>0.3</sub> Ga <sub>0.7</sub> As	GaAs:p	GaAs:n	Al <sub>0.5</sub> ln <sub>0.5</sub> P
Thickness(µm)	2.00	3.50	0.12	0.02
Bandgap(eV)	1.8	1.42	1.42	2.4
Dielectric constant	11.56	13.18	13.18	10.00
Electron affinity(eV)	3.74	4.07	4.07	4.50
$N_c(1/cm^3)$	1.00E+19	4.70E+17	4.700E+17	1.00E+19
$N_V(1/\mathrm{cm}^3)$	1.00E+19	7.00E+18	7.00E+18	1.00E+19
$V_e(\text{cm/s})$	1.00E+7	1.00E+7	1.00E+7	1.00E+7
$V_h(\text{cm/s})$	1.00E+7	1.00E+7	1.00E+7	1.00E+7
$\mu_e$ (cm <sup>2</sup> /Vs)	5.00E+2	4.70E+3	8.60E+2	1.00E+2
$\mu_e$ (cm <sup>2</sup> /Vs)	6.00E+1	3.00E+2	1.50E+2	1.00E+1
$N_D(1/cm^3)$	1.00E+15	0.00E+00	2.00E+18	8.00E+18
$N_A(1/cm^3)$	2.00E+18	9.00E+16	0.00E+0	1.00E+15

Table 2-5 Electrical parameters corresponding to different layers regarding simulation of GaAs solar cell

### 2.4.1 Result of simulation of GaAs solar cell



Figure 2.9 Energy versus position band diagram of the GaAs cell at (a) dark and (b) illuminated condition

A reference fermi level is at 0.00eV and a defect state highlighted with green colour is at 0.71eV above the reference valence band in dark equilibrium at no bias, in illuminated conditions  $V_{OC}$  is given by the splitting between quasi-fermi levels.

The spectral utilization of the solar cell that is measured in terms of QE is depicted in Figure 2.10(b) and the characteristics J-V curve of the simulated solar cell have been depicted in Figure 2.10(a).



Figure 2.10 (a) J-V curve of the GaAs cell (b) Spectral utilization of the GaAs cell

#### The derived external parameters are presented in Table 2-6.

Table 2-6 Extracted external parameters of GaAs solar cells

External Parameters	V <sub>oc</sub> (volt)	$J_{SC}(mA/cm^2)$	<b>FF</b> (%)	<b>PCE</b> (%)
Simulated result	1.0218	25.91	87.78	23.24

### 2.5 Simulation of Ge-based Solar Cell

The structure that has been opted for the simulation is taken from the reference[36], a schematic diagram is depicted in Figure 2.11. The technique of the simulation is very similar to what we have done previously, the study of various parameters of different layers has been tabulated in Table2-7. Losses

associated with the device are radiative recombination coefficient  $1.00\text{E}-10(\text{cm}^3/\text{s})$ . As far as optical losses are concerned the reflection of 10% from the front surface has been taken into consideration.



Figure 2.11 Ge cell structure

Table 2-7 Electrical parameters corresponding to different layers regarding simulation of Ge solar cell[36]

Parameters	Ge:p	Ge:n	InGaP
Thickness(µm)	180	0.180	0.98
Bandgap(eV)	0.664	0.664	1.82
Dielectric constant	16.00	16.00	10.00
Electron affinity(eV)	4.00	4.00	4.50
$N_{C}(1/\mathrm{cm}^{3})$	1.040E+19	1.040E+19	1.00E+19
$N_V(1/\mathrm{cm}^3)$	6.00E+18	6.00E+18	1.00E+19
$V_e(\text{cm/s})$	1.00E+7	1.00E+7	1.00E+7
$V_h$ (cm/s)	1.00E+7	1.00E+7	1.00E+7
$\mu_e(\mathrm{cm}^2/\mathrm{Vs})$	2.60E+3	1.00E+3	8.03E+2
$\mu_h(\mathrm{cm}^2/\mathrm{Vs})$	7.00E+2	1.00E+2	4.00E+1
$N_D(1/cm^3)$	0.00E+00	8.50E+18	3.00E+18
$N_A(1/cm^3)$	1.50E+17	0.00E+00	0.00E+0

#### 2.5.1 Result of simulation of Ge solar cell

Looking at the J-V curve, a high short circuit current nearly 40mA/cm<sup>2</sup> is obtained due to the absorption of low as well as high energetic photons because Ge has a smaller band gap. At the same time, we have a small open-circuit voltage of around 0.26 volts because the extent of splitting between quasi-fermi levels is much less due to the smaller band gap.



Figure 2.12 (a) J-V curve of the GaAs cell (b) Spectral utilization of the Ge cell

Table 2-8 Extracted external parameters of GaAs solar cells

External Parameter	$V_{oc}(V)$	$J_{sc}(mA/cm^2)$	<b>FF</b> (%)	<b>η</b> (%)
Simulated result	0.26	40.88	69.17	7.36

### 2.6 Summary

It is confirmed by performing simulations on various single junction photovoltaic technologies such as homojunction solar cells based on GaAs and Ge absorber material, heterojunction solar cells based on CdTe absorber material, perovskite solar cells based on CsGeI<sub>3</sub> absorber material, that the open-circuit voltage( $V_{oc}$ ) is determined by the extent to which the quasi-fermi level  $E_{Fn}$  and  $E_{Fp}$  are able to split. The splitting of the quasi-fermi level is limited by the recombination mechanism due to the presence of the defect in the solar cell, which leads to a deficit in open-circuit voltage.

## Chapter 3 <u>-Influence of midgap states on the photovoltaic</u> performance: A case study with numerical simulation

#### **3.1 Introduction**

In this chapter reader's attention is brought towards the serious loss mechanism(recombination of optically generated charge carrier) occurring in the device, which categorizes into two, first one is unavoidable and cannot be controlled includes spontaneous radiative recombination and Aguer recombination, unlike radiative recombination is dominant in direct band gap material, Auger recombination is dominant in both direct as well as indirect band gap material because it is a threeparticle process which conserves both energy and momentum, e.g. auger recombination is still dominant loss occur in high grade pure single crystalline solar cell. Another one is avoidable i.e. that can be controlled by the manufacturing process, like defects present in the solar cell can be further reduced by applying different synthesis approaches. The presence of this electronic defect definitely obstructs the carrier transport mechanism which results in a decrease in device performance. It is widely recognized that the overall structural disorder present in the semiconductor is measured in terms of Urbach energy  $(E_U)$  which reflects in the formation of tail states near the band edges in the forbidden band gap of the semiconductor [1], [37], [38], [39], [40]. Since the Urbach energy is a measure of the electronic disorder and can impart information of the cell performance[41]. one of the approaches for investigating loss mechanism in solar cells involves the study of Urbach energy  $(E_U)$  as a diagnostic parameter [42]. One of the main external parameter that directly affects the others is open-circuit voltage( $V_{0C}$ ), Hence, using simulation methodology, investigations into the variation of open-circuit voltage with Urbach energy have been performed. In this study, we restrict ourselves to the variation in defect concentration only and show how this affects the external parameters of the solar cell. Hence by using an alternative numerical simulation methodology, we will demonstrate the bijective correspondence between opencircuit voltage( $V_{oc}$ ) and Urbach energy( $E_U$ ). Such a study can contribute to the fundamental understanding of the solar cell materials. In this study, we take the support of thin-film technology cadmium telluride (CdTe) because thin-film photovoltaic solar cells are seen to be among the most promising solar cells because of their high energy conversion efficiency, affordability, and ease of largescale manufacturing.

#### 3.2 Method

The presence of defects in semiconductors leads to the formation of defect energy levels within the forbidden region which facilitates a non-radiative SRH(Shockley Read Hall) recombination. Depending upon their position in the forbidden region these defect states may act as trap or recombination centers[1]. Mathematical expression for the recombination rate( $U_{SRH}$ ) is given by[43].

$$U_{SRH} = \frac{np - n_i^2}{\tau_{n,SRH}(p + p_t) + \tau_{p,SHR}(n + n_t)} \qquad \dots 3.1$$

Where n and p are electron and hole concentrations in conduction and valance bands respectively,  $n_i$  is intrinsic charge carrier density,  $\tau_{p,SHR}$  and  $\tau_{n,SRH}$  are the lifetimes of holes and electrons which are inversely proportional to defect concentration,  $n_t$  and  $p_t$  are the value of the electron density and hole density respectively when the electron Fermi level is equal to the trap level given by the expression.

$$n_t = n_i e^{(E_t - E_i)/k_B T}$$
 ... 3.2

$$p_t = n_i e^{(E_i - E_t)/k_B T} \qquad \dots 3.3$$

Here  $E_i, E_t$  and  $k_B$  are intrinsic energy level, trap energy level, and Boltzmann constant respectively. From equation 3.1 one can observe that recombination depends on defect concentration and from equations 3.2 and 3.3 it should be important to note that the quantities  $n_t$  and  $p_t$  are parameters that introduce the dependency of the recombination rate on the trapping energy level  $E_t$ . It is known that the signature of total structural disorder within the system including the information of the defects can be drawn in terms of the evolution of Urbach energy of the system[44]. Therefore, an explicit quantitative analysis between Urbach energy  $(E_U)$ , defect concentration in the active layer and open-circuit voltage( $V_{oc}$ ) can provide a useful insight into solar cell materials which can be helpful in comprehending the overall performance based on the initial optical characterizations. In that view, the numerical simulation methods have been helpful for researchers; although such tools are primarily utilized to optimize a cell structure knowing the internal parameters of various layers, however, its potential to comprehend the role of the Urbach energy on the midgap states in the cell performance should not be ignored. Therefore, in the current, we consider a cell device structure using the SCAPS-1D software and perform numerical simulation for the defect concentrations in the active layer thereby connecting it with the evolution of the Urbach energy and ultimately with the output parameters of the photovoltaic cell. In the scenario of nearly consistent reflectance from the solar cells, EQE in longerwavelength edges can be expressed as [45], [46].

$$\ln(EQE) = \frac{hv}{E_{II}} + C \qquad \dots 3.4$$

Where hv is the photon energy and *C* is constant whereas the inverse slope of equation 17 quantifies the Urbach energy( $E_U$ ). As above explained loss of charge carriers via non-radiative recombination (SRH) depends on two factors the defect concentration and the position of the defect level in the forbidden zone of the band gap.

The procedure that we follow keeps the defect level at a fixed position and varies defect density for absorber layer CdTe and observes the effect of bulk recombination current(J\_SRH), along with the external parameters of the solar cell and finally shows that there is one to one correspondence between Open-circuit voltage( $V_{oc}$ ) and Urbach energy( $E_U$ ).

#### 3.3 Result and Discussion

#### 3.3.1 Variation of external parameters with respect to defect density

The solar cell structure that we simulated for this study is CdTe/CdS the details of simulated parameters and the result of the simulation are presented in chapter2 in the section2.3.

We will observe the effect on external parameters of the solar cell with an increase in the neutral defect density of the absorber material which varied in the range from  $1.00 \times 10^{17} cm^{-3}$  to  $1.00 \times 10^{19} cm^{-3}$  which is consistent with the literature[47].

Before proceeding with the external parameters plot, it is essential to plot the Shockley-Read-Hall recombination current density (J\_SRH) against the voltage across the solar cell for each specific defect

density. This preliminary step will allow us to observe and analyze the extent of variation in J\_SRH corresponding to different defect densities.



Figure 3.1 SRH recombination current density vs Bais voltage across solar cell when the defect density are varied from  $1.00 \times 10^{17} \text{ cm}^{-3}$  to  $1.00 \times 10^{19} \text{ cm}^{-3}$ 

From Figure3.1 one can observe that the photo-generated current is constant and does not vary with change in defect density and voltage across the solar cell, as defect density increased from  $1.00 \times 10^{17}$  cm<sup>-3</sup> to  $1.00 \times 10^{19}$  cm<sup>-3</sup> the value J\_SRH recombination current increases irrespective of the value of voltage across the solar cell. The voltage where J\_SRH recombination current density exceeds the photo-generated current density, the solar cell instead of generating power, starts consuming the power.





Figure 3.2 (a)  $V_{OC}$  (b)  $J_{SC}$  (c) FF, and (d) PEC variation with respect to defect density.

Here we observe that the V<sub>OC</sub> decreases with an increase in the defect density starting with defect density  $1.00 \times 10^{17}$  cm<sup>-3</sup> when V<sub>OC</sub> is 0.5001 volt it diminishes to 0.2884 volts when defect density is  $1.00 \times 10^{19}$  cm<sup>-3</sup>. This reduction in V<sub>OC</sub> is due to the fact that with a continuous increase in the defect density the recombination of charge carriers increases due to this the lifetime of optically generated charge carriers reduces hence diffusion length, reducing the probability of collection of charges at the front and the back contacts. Which results decline in V<sub>OC</sub>. J<sub>SC</sub> also decreases with increases in the defect density, because the defects provide an alternative recombination path within the solar cell, which means a significant amount of optically generated charge carriers recombine before getting collected to the back and front contact. The FF increases due to the increase in the "squareness" of the J-V curve, the power conversion efficiency(eta) should also decrease due to the loss of optically generated charge carrier via recombination.

#### 3.3.2 Effect on Urbach Energy due to increase in the defect density

The reciprocal of the slope of Equation 3.4 yields the Urbach Energy. It is noteworthy that this expression is applicable within the longer wavelength region. Consequently, to determine the Urbach energy, consideration is given to the EQE points situated below the bandgap.





Figure 3.3 Plots of In(EQE) v/s Photon Energy(eV) at various defect concentration

With a similar approach Urbach energy can be found for each defect concentration, the outcomes are tabulated in Table3-1.

Table 3-1 Variation of Urbach energy and or	pen-circuit voltage with defect densit	y
---	--	---

Defect Density(cm <sup>-3</sup> )	Urbach Energy(meV)	Open-circuit voltage(volt)
$1.00 \times 10^{17}$	20.8006	0.50011
$5.00 \times 10^{17}$	20.8507	0.40897
$1.00\times10^{18}$	21.1278	0.37512
$5.00 \times 10^{18}$	23.0994	0.31153
$1.00 \times 10^{19}$	24.5415	0.28842

Graphical representations depicting the relationship between Urbach energy and open-circuit voltage with respect to defect density are illustrated below.



Figure 3.4 (a) Drop in V<sub>oc</sub> with respect to Urbach energy (b) Variation in Urbach energy with an increase in defect concentration

Open-circuit voltage decreases rapidly with an increase in Urbach energy, according to Figure 3.4(a) value of open-circuit voltage decreases from 0.5 volt to 0.28 volt with an increase in Urbach from 20.80 meV to 24.5 meV. From Figure 3.4 (b) Urbach energy increases with an increase in defect density a significant increase in Urbach energy has been observed when defect density increases beyond 1E+18 cm<sup>-3</sup>.

### 3.4 Summary

This chapter explores how external parameters change with varying defect densities in solar cells. Further, employing an empirical mathematical relationship demonstrates that as the defect concentration increases, the Urbach energy also rises.

## Chapter 4 -Device Optimization

#### **4.1 Introduction**

In the previous chapter we have dealt with the loss mechanism occurring within the solar cell, now apart from the loss mechanism, a study has been performed towards optimizing the generation mechanism, in the ever-changing world of renewable energy, Fine-tuning the fabricated solar cell device becomes important to use the full potential of renewable energy, optimizing the solar cell is not an easy task as the performance of the device is affected by the several parameters, to do optimization we have to take the support of the computation method and to make computation easy there are various extraordinary simulator tools which enveloped with numerous mathematical models where numerical simulations can be performed with enhanced accuracy help to understand device response under several initial conditions, Scaps-1D has potential to filter out best-optimized device. In this section refinement of the perovskite solar cell (CsSnCl<sub>3</sub> absorber material) has been carried out by varying absorber doping strength, HTL, ETL, and absorber thickness.

#### 4.2 Cell Description

The design of the cell is depicted in Figure 4.1, fullerene is used as ETL, and Cu<sub>2</sub>BaSnS<sub>4</sub> works as HTL. The electrical parameters of the various sandwiched layers are illustrated in Table 4-1, back contact work function is taken to be 5.1 eV. The result of the simulation has been illustrated in Table 4-2, a  $V_{OC}$  of 1.00 volt,  $J_{SC}$  of 21.16 mA/cm<sup>2</sup>, FF of 77.69% and PCE of 16.47% were reported initially before optimization.



Figure 4.1 Schematic Cell Structure

### 4.3 Optimizing ETL

ETL plays a crucial role in enhancing the PEC of the device by facilitating the extraction and transportation of electrons from the light-absorbing layer to the electrode, minimizing losses due to recombination. Initially, an ETL thickness of 100nm is introduced, to optimize, ETL thickness ranging from 25nm to 450nm is taken into consideration. From Figure 4-2(b), an Increment in the value of  $J_{SC}$  has been observed from 21.16 mA/cm<sup>2</sup> to 25.74mA/cm<sup>2</sup> with the decrease in the ETL thickness starting from 100nm to 30 nm(not visible in Figure 4-2 due to higher scale of the x-axis for convenience the data will be provided in Appindix1) and a small increment in voltage has also been observed, which

overall increases the PCE of the device, the decrease in the device performance with increase the thickness of ETL is due to the exponential decay of the injected excess electron in the ETL, even this could be visualized in more quantitative approach by solving differential diffusion equation for the electron under a steady condition which simplifies to Equation 4.1(see Appindix2).

$$\delta_n(x) = \Delta n e^{\left(-x/L_n\right)} \qquad \dots 4.1$$

Where,  $\delta_n(x)$  the concentration of electrons measured at any position x,  $\Delta n$  is the concentration of injected electron at position x = 0,  $L_n$  is the diffusion length. The optimized thickness of the ETL comes out to be 30nm.

Parameter	ΙΤΟ	ETL	Absorber	HTL
Thickness(nm)	500	100	700	100
$E_g(eV)$	3.5	1.7	1.52	1.9
$\chi_e(eV)$	4	3.9	3.90	3.6
$\boldsymbol{\varepsilon}_r$	9	4.2	29.4	5.4
$N_{C}(cm^{-3})$	$2.2 \times 10^{18}$	$8.0 \times 10^{19}$	$1.0 \times 10^{19}$	$2.2 \times 10^{18}$
$N_V(cm^{-3})$	$1.8 \times 10^{19}$	$8.0 \times 10^{19}$	$1.0 \times 10^{19}$	$1.8 \times 10^{19}$
$\mu_e$ (cm <sup>2</sup> /Vs)	20	$8.0 \times 10^{-2}$	2	30
$\mu_h$ (cm <sup>2</sup> /Vs)	10	$3.5 \times 10^{-3}$	2	10
$N_A(cm^{-3})$	0	0	$1.0 \times 10^{14}$	$1.0 \times 10^{18}$
$N_D(cm^{-3})$	$1.0 \times 10^{21}$	$1.0 \times 10^{17}$	0	0
$N_t(cm^{-3})$	$1.0 \times 10^{15}$	$1.0 \times 10^{15}$	$1.0 \times 10^{15}$	$1.0 \times 10^{15}$

Table 4-1 Initial material parameter for Scaps 1-D

Table 4-2 Extracted external parameters

External Parameter	$V_{oc}(V)$	$J_{sc}(mA/cm^2)$	<b>FF</b> (%)	η(%)
Simulated result	1.00	21.16	77.69	16.47





Figure 4.2 Variation of (a)Voc, (b)JSC, (c)FF and (d)PEC with ETL thickness



#### **4.4 Optimizing HTL**

Figure 4.3 Variation of (a) Voc, (b) J<sub>SC</sub>, (c) FF, and (d) PEC with HTL thickness

HTL facilitates the movement of holes within the solar cell, how HTL works in the collection of holes from the absorber layer and exporting to the contact can be explained with the help of the energy versus position band diagram, the same has been done in the section 2.2.3, initially, the thickness of the HTL was taken to be 100nm, to optimize, HTL thickness ranging from 50nm to 500nm is taken into consideration. All the external parameters remain almost unchanged with the variation in HTL thickness, this means that there is negligible recombination or we can say that there is no decay of the

injected hole in the HTL because HTL is highly acceptor dopped which increases the lifetime of the hole and hence the diffusion length which leads to negligible recombination(see Equation 4.1). Overall the HTL thickness does not affect the performance of the device, hence taking an initial value of HTL as optimized.

### 4.5 Optimizing Absorber

The absorber layer plays a very crucial role in converting sunlight directly into electricity by absorbing photons, Researchers continually putting efforts to enhance absorber materials to improve efficiency, reduce costs, and make solar energy more competitive with other forms of electricity generation. Initially, the thickness of the absorber layer of 700nm was introduced, to optimize further, the absorber thickness ranging from 500nm to 2000nm was taken into consideration.



Figure 4.4 Variation of (a) V<sub>OC</sub>, (b)J<sub>SC</sub>, (c) FF, and (d) PEC with absorber thickness

A continuous decrement in the  $V_{OC}$ , Starting from 1.01 volt to 0.95 volt has noticed with increase in the thickness of the absorber layer from 500nm to 2000nm. Variation of other three external parameters with absorber thickness is same, first increases continuously and then attain maximum at some point and then decreases gradually. The J<sub>SC</sub> attains its maximum value at 1200nm, The FF attains its maximum value at 700nm, and the PEC attains its maximum value at 800nm, the optimized thickness of the absorber layer is 800nm.

Initially, with an increase in the thickness of the absorbing material, the absorption of photons increases resulting in a significant increase in generated charge carriers as a consequence the  $J_{SC}$  increases significantly this trend will follow up to some extinct, after the further increase in the thickness of the

absorbing material the value of the  $J_{SC}$  decreases significantly due to recombination of generated minority charge carrier because now the diffusion length of the minority carrier is much less than the thickness of absorbing material. Increasing the thickness beyond the limit gives two more negative factors which include an increase in series resistance and a lower band gap of the absorber material.

#### 4.6 Optimizing Absorber acceptor concentration

Doping, in the context of the absorber layer, involves intentionally introducing specific impurities into the semiconductor material to modify its electrical properties. This process plays a crucial role in enhancing the performance and efficiency of the solar cell. initially, the acceptor concentration of  $1.0 \times 10^{14}$  cm<sup>-3</sup> is introduced in the absorber layer. To optimize, a simulation ranging from  $0.0 \times 10^{00}$  cm<sup>-3</sup> to  $1.0 \times 10^{18}$  cm<sup>-3</sup> is performed. The result of the simulation is illustrated in Figure 4-5.



Figure 4.5 Variation of (a) $V_{OC}$ , (b)  $J_{SC}$ , (c) FF, and (d) PEC with absorber acceptor density

The V<sub>oc</sub> remains constant up to variation in doping density  $1.0 \times 10^{14}$  cm<sup>-3</sup> and, increases significantly as doping concentration increased beyond  $1.0 \times 10^{15}$  cm<sup>-3</sup> due to change in band alignment with doping, the FF remains almost constant up to defect concentration of the  $1.0 \times 10^{13}$  cm<sup>-3</sup> beyond this it starts increasing and attains maximum value of 77.94% at doping of the level  $1.0 \times 10^{15}$  cm<sup>-3</sup> after that FF drops rapidly with increase in the defect concentration and finally it reduces to 72% when the doping concentration is  $1.0 \times 10^{18}$  cm<sup>-3</sup>, in the case of J<sub>SC</sub> and PCE a similar trend was observed, J<sub>SC</sub> and PCE remains constant up to the doping concentration of  $1.0 \times 10^{14}$  cm<sup>-3</sup> and further increases significantly, the J<sub>SC</sub> attains maximum value of 22.91 mA/cm<sup>2</sup> when doping density was  $1.0 \times 10^{16}$  cm<sup>-3</sup>, and shows a nearly constant behaviour up to doping density  $1.0 \times 10^{17}$  cm<sup>-3</sup>, and after that it drops rapidly to 19.56 mA/cm<sup>2</sup> when doping density was  $1.0 \times 10^{19}$  cm<sup>-3</sup>, in similar fashion PEC attains the maximum value of 18.24% when the doping density was  $1.0 \times 10^{17}$  cm<sup>-3</sup> and after that it drops rapidly to 16.06% when the doping density was  $1.0 \times 10^{19}$  cm<sup>-3</sup>, keeping in mind that we have a high V<sub>OC</sub>, J<sub>SC</sub> and at the same time we do not lose FF much, the optimized value of the absorber acceptor doping is  $1.0 \times 10^{16}$  cm<sup>-3</sup>.

To understand the reason behind the behaviour of PEC with doping density, Initially, let's consider that our absorber material is undoped, then in this situation we found that the PEC is minimum(see data provided in Appindix1) because in undoped material the non-radiative recombination(SRH recombination) is maximum, when the concentration of the holes and electrons are equal, this can be visualized from the Equation 4.2,  $U_{SRH}$  (rate of recombination) will be maximum when n = p.

$$U_{SRH} = \frac{np - n_i^2}{\tau_{n,SRH}(p + p_t) + \tau_{p,SHR}(n + n_t)} \qquad \dots 4.2$$

Hence, the doping, of the absorber layer, will reduce non-radiative losses(SRH recombination) as well as increase the conductivity of the material, but high doping levels result in the reduction of the device performance because as the doping level increases the lifetime of the minority carrier decreases which results in the significant loss of the generated charge carriers.

### 4.7 Summary

After implementing the optimization techniques, significant enhancements were observed in several critical aspects of the solar cell's performance. The optimized design resulted in a  $V_{OC}$  of 1.04 volt,  $J_{SC}$  of 26.12 mA/cm<sup>2</sup>, FF of 82.28% and PEC of 22.49% same has been tabulated in Table4-3. The corresponding J-V curve is depicted in Figure 4-6.



Table 4-3 Result of Optimized solar cell

Figure 4.6 J-V curve of optimized Cell

# Chapter 5 -Simulation of multi-junction solar cell

### **5.1 Introduction**

Scaps-1D is a well-known simulator tool as far as the simulation of single junction solar cells is concerned, however, its latest version is equipped with software script support. This new update enables users to simulate multijunction and tandem solar cells, the procedure is not as straightforward as experienced in single junction, first, you have to explicitly architect individual single junction solar cells and last you have to connect them in series using script support. Starting with Shockley Quisser-limit for single junction solar cells we step towards multijunction solar cells which is a way to overcome this limit. The importance of different layers such as the window layer, back surface field, and tunnel junction has been enveloped in this chapter.

## 5.2 Shockley-Queisser limit

As far as single junction solar cell is concerned the two main external parameters of the solar cell i.e.  $V_{OC}$  and  $J_{SC}$  their maximum theoretical limit is influenced by the band gap of the material, Thus, within the realm of single-junction solar cells, the question arises, what is the optimal band gap for the absorber semiconductor to achieve the highest conversion efficiency under the A.M. 1.5 solar spectrum?

## 5.3 Spectral Utilization

QE is a parameter that quantifies the spectral utilization in solar cells, The device converts different portions of the solar spectrum, primarily sunlight, into electricity depending on the band gap of absorber material. Solar cells are designed to capture photons and convert their energy into electrical current. In order to get better efficiency, we have exploited as much as possible part of the solar spectrum. Now will see the spectral utilization by two different absorber materials whose band gap is comparatively small and comparatively large.

### 5.3.1 Effect of spectral utilization on the material whose band gap is comparatively large

To analyze the impact of spectral utilization in high band gap materials, a simulation was conducted on gallium arsenide (GaAs) based solar cells whose band gap is 1.42 eV. The simulated cell structure is illustrated in Figure 5.1.



Figure 5.1 Schematic representation of GaAs cell

This solar cell structure has been already simulated in chapter2 the result of the simulation has been directly used. From Figure 5.2 (a) it should be noted that an open circuit voltage of 1.02 volts has been obtained with the short circuit current density of  $25.91 \text{ mA/cm}^2$ . The Spectral utilization of solar cell can be predicted from Figure 5.2 (b) photons having energy higher than band gap energy participate in electron-hole pair generation.

Predominantly shorter wavelength part i.e. below 850nm spectrum has been utilized successfully. Due to again recombination of optically generated charge carrier's quantum efficiency has been reduced below 85%, and a slightly lower QE has been figured out below 520nm this is due to the absorption of higher energy photons takes place in the window layer(front layer) and due to low mobility of hole, generated minority charge carrier(hole) recombine again.



Figure 5.2 (a) J-V curve of GaAs cell (b) Spectral Utilization of the GaAs cell

### 5.3.2 Effect of spectral utilization on the material whose band gap is relatively low

Investigating the impact of spectral utilization in low band gap materials, a simulation was conducted on germanium-based solar cells with a band gap of 0.66 eV. The simulated cell structure is illustrated in Figure 5.3.



Figure 5.3 Simulated Ge cell

The result of the simulation directly imported from chapter2, an open-circuit voltage of around 0.26 volt and a short-circuit current density of 40mA/cm<sup>2</sup> has been obtained, spectral response can be interpreted from Figure5.4(b), since the band gap of absorber material is relatively small so the absorption spectrum will shift towards higher wavelength region, which reflected very well in QE curve (lower energy photons efficiently participate in electron-hole pair generation). It is noteworthy that the QE for lower wavelength regions below680nm is significantly lower because higher energy photons have low penetration depth and get absorbed within the window layer (front layer), most of the

generated minority charge carrier(hole) will again recombine due to its low mobility as a result generated carrier do not get collected at the back contact responsible for lower QE for higher energy photons.



Figure 5.4 (a) J-V curve of Ge cell (b) Spectral utilization of the Ge solar cell

### 5.4 A comparative study of materials having a relatively higher and lower band gap

#### 5.4.1 J-V curve

The characteristic J-V curve of both GaAs solar cell and the Ge solar cell has been illustrated in Figure 5.5.



Figure 5.5 J-V curve of both materials (a) blue curve reflects the J-V curve of Ge solar cell which has a lower band gap (b) red curve reflects the J-V curve of GaAs solar cell which has a higher band gap

✤ J-V curve of GaAs solar cell: -

▶ High  $V_{OC}$ .

- $\blacktriangleright$  Relatively low  $J_{SC}$  is obtained.
- ✤ J-V curve of Ge solar cell: -
  - $\succ$  Low  $V_{OC}$ .
  - > Relatively high  $J_{SC}$  is obtained.

A high  $V_{OC}$  in the case of GaAs solar cell is a consequence of its high band gap which leads to splitting in quasi fermi level to higher extinct, on the other hand, having low short circuit current density because only higher energy photon participates in electron-hole pair generation. In the case of Ge solar cell smaller band gap is responsible for having low  $V_{OC}$  due to less splitting in quasi-fermi level and high short circuit current density.

### 5.4.2 spectral utilisation



Figure 5.6 QE curve of both materials (a) red curve reflects the QE curve of Ge solar cell which has a lower band gap (b) blue curve reflects the QE curve of GaAs solar cell which has a relatively large band gap

- Spectral Utilization of GaAs solar cell relatively high band gap material: -
  - From Figure 5.6 it is clear that the photons that are below the band gap do not participate in the generation of electron-hole pair.
  - > The EQE is negligible for the wavelength larger than 880 nm.

- > The part of the spectrum that is beyond 880nm is not utilized.
- Spectral Utilization of Ge solar cell relatively low band gap material: -
  - > The part of the spectrum that is beyond 1880nm is not utilized.
  - > Ge solar cells efficiently harness the solar spectrum from 680nm to 1880nm.

Higher band gap material uses only the lower wavelength part of the spectrum and lower band gap material uses only the higher wavelength part of the spectrum much more efficiently. This puts the upper limit on the power conversion efficiency of the single junction solar cell, well known as the Shockley-Queisser limit[43]. To exploit as much as possible part of the solar spectrum one has to go with the multijunction solar cell.

### 5.5 Multijunction Solar cell

In a multijunction solar cell/Tandem, there is the stacking of 2-3 different junctions of solar cell one over another to exploit the much more part of the solar spectrum, The typical configuration of a multijunction solar cell is presented below in Figure 5.7.



Figure 5.7 Schematic representation of Multijunction solar cell

The architecture of a multijunction solar cell depends on the penetration depth of the wavelength, The spectral portion corresponding to the most energetic photons, such as blue light, exhibits the shortest penetration depth within materials, consequently, the highest band gap junction always functions as the top cell, similarly the spectral segment corresponding to the less energetic photon, such as near-infrared, exhibits the larger penetration depth within the materials, as a consequence the smallest band gap junction always functions as the bottom cell, the same has been illustrated in Figure 5.7.

Now, we will explore the significance of the various layers used in the cell structure.

### 5.5.1 Window layer

Surface termination leads, to unsatisfactory bonding to the exposing atom, resulting formation of dangling bonds, and as a consequence leads to the formation of defect levels in position versus the energy band diagram near the surface which facilitates optically generated charge carriers to recombine via transferring heat to the lattice. Growing a window layer on top of it will partially restore the bonding environment, and reduce the loss of generated carrier, to prevent optical losses due to absorption within the window layer it is practiced to select material with a high band gap and at the same time its lattice parameter should also be matched with the layer on top of that we want to grow. Further, the function of the window layer can be summarised in two points.



Figure 5.8 Energy v/s position band diagram of the first cell

- Provides good passivation to prevent Surface recombination.
- Provide selective contact, from Figure 5.8 the generated charge carrier electron will tunnel through a small barrier due to the formation of heterostructure between the absorber and the window layer at the same time hole encounters a high barrier and reflects back which prevents the recombination of generated charge carrier.

### 5.5.2 Back Surface Field

In reference to Figure 5.8 AlGaInP works as a back surface field which is highly p dopped, similar to the window layer BSF also provides surface passivation and selective contact, the generated charge carrier hole gets easily collected to the back contact as it does not face any potential barrier, but at the same time, electron encounters a huge potential barrier and reflected back which prevent recombination of generated charge carrier.

### 5.5.3 Tunnel Junction

Tunnel junction plays a crucial role in the operation of multijunction solar cells by providing electrical connection and current matching between the subcells. The absence of tunnel junction causes electrical resistance and voltage drop this can be easily understood by considering the simple assumption of stacking consecutively three p-n junctions one another illustrated in Figure 5.9.



Figure 5.9 Stacking of the p-n junction without tunnel junction

Considering the flow of current in the vertically upward direction, junctions 1,3 and 5 are in forward bias but at the same time junctions 2 and 4 are in reverse bias, hence junctions 2 and 4 limit the magnitude of current flowing through the device because in reverse bias current flow due to drift of minority charge carrier, which is limited by the thermally generated minority charge carrier, which is main cause for electrical resistance and voltage drop.

By adding a tunnel junction, it is possible to stop the development of this kind of reverse bias junction.

- It offers minimal electrical resistance.
- Additionally, it has a large band gap to stop losses from parasitic absorption.

Before exploring the operation of multijunction solar cells, let's discuss the properties of tunnel junction that make tunnelling favourable, degenerate semiconductor materials are used i.e. in n-type material fermi level lies above the conduction band, and in p-type material, fermi level lies below the valence band this can be clearly pointed out in Figure 5.10 in the region of the tunnel junction. High doping also responsible for a narrow depletion zone which increases the probability of tunnelling because tunnelling probability depends on the width (not height) of the potential barrier, the higher the potential width lower will be the tunnelling probability.



Figure 5.10 Energy v/s position band diagram of the first cell with tunnel Junction

In order to explain the operation of a multijunction solar cell with tunnel junction energy versus position band diagram has been simulated and illustrated in Figure 5.10, at the right of the tunnel junction energy versus position band diagram corresponds to the top cell, and the left of the tunnel junction energy versus position band diagram corresponds to the middle cell, generated electrons in the middle cell will recombine with the generated holes of the top cell, similarly generated electrons of the bottom cell will recombine with the generated holes of the middle cell, this demonstrates that recombination current at the tunnel junction represents the current density of the triple junction solar cells. That's why, the cell which is producing the lower current will determine the current density of the cell. keeping all the aforementioned discussed ideas about multijunction solar cells now we are stepping towards the simulation of a simple two-junction solar cell using Scaps-1D by using script support.

#### 5.6 Method of Simulation

Here we use the GaAs solar cell (structure represented in Figure 2.8) as the top cell and the Ge solar cell (structure represented in Figure 2.11) as the bottom cell. The strategy that we use to simulate the two junction Tandem cell using SCAPS-1D is that first we separately design the top cell (GaAs) and separately bottom solar cell (Ge), to combine them in series connection followed by the extraction of the resultant J-V curve of the tandem solar cell along with external parameters we use SCAPS-1D script.

Assumption: -

• Ideal tunnel junction.

- The spectrum that is utilized by the top cell will correspond to that region for which photon energy is higher than the band gap of the top cell.
- The spectrum that is utilized by the bottom cell will correspond to the part of the spectrum that is unabsorbed by the upper absorber layer and also, we considered that some part of the spectrum is transmitted without absorption (20%).



Figure 5.11 Two Junction Tandem cell

### 5.7 Scaps-1D script execution procedure

Step 1: write your script in any platform such as Notepad and save the file in the provided Scaps-1D library script folder with the file extension(.script).

Step 2: Set working conditions such as temperature, upload spectrum file according to requirement, stop voltage, and select the action that you want to perform.

SCAPS 3.3.10 Action Panel				– 🗆 X
Working point     \$300.00       Temperature (K)     \$0.0000       Voltage (V)     \$0.0000       Frequency (Hz)     \$1.000E+6       Number of points     \$5	Series resis	As Ohm.cm <sup>2</sup> 2 Rsh #1.00E+3 S/cm <sup>2</sup> 2 Gsh #1.00E-3	Action list Load Action List Save Action List	All SCAPS settings
Illumination: Dark Li Analytical model for spectrum Spectrum file name: illumi Select	ght Specify i Spectrum from file nated from left illuminate	illumination spectrum, then calculate G(x)	Directly specify G(x) Analytical model G(x) model	for G(x) G(x) from file
spectrum file Spectrum cut off? yes Neutral Density \$0.0000	AM1_5G Short wavel. (nm) 🚆 200.0 Long wavel. (nm) 🚆 4000 Transmission (%) 💭 100.0	1 sun.spe         sun or lamp         1000.00           after cut-off         1000.00           000         after ND         1000.00	Ideal Light Current Transmission of att Ideal Light Current	tin G(x) (mA/cm2) 20.0000 tenuation filter (%) 100.00 tin cell (mA/cm2) 0.0000
Action Pa	use at each step		number	
⊫ <sub>I-V</sub>	V1 (V) 📥 0 0000	V2 (V) 🔺 1 5000	of points	0.0200 increment (V)
	V1 (V) 0.0000 V1 (V) 0.8000 f1 (Hz) 1.000E+2	V2 (V) \$1.5000	of points 76 81 21	0.0200 increment (V) 0.0200 increment (V) 5 points per decade
<ul> <li>F</li> <li>F</li> <li>C-V</li> <li>F</li> <li>C-f</li> <li>F</li> <li>QE (IPCE)</li> </ul>	V1 (V) ♥ 0.0000 V1 (V) ♥ -0.8000 f1 (Hz) ♥ 1.000E+2 WL1 (nm) ♥ 300.00	V2 (V) \$1.5000 V2 (V) \$0.8000 f2 (H2) \$1.000E+6 [WL2 (nm)] \$200 00	of points after Voc 276 2 811 2 21 2 171 2	0.0200 increment (V) 0.0200 increment (V) 5 points per decade 10.00 increment (nm)
	V1 (V) \$0.0000 V1 (V) \$-0.8000 f1 (Hz) \$1.000E+2 WL1 (nm) \$300.00 loaded definition file:	V2(V) \$1.5000	of points after Voc 276 2 21 2 171 2 Problem file: new problem	0.0200     increment (V)       0.0200     increment (V)       5     points per decade       10.00     increment (nm)
	V1 (V) \$0.0000 V1 (V) \$0.8000 f1 (H2) \$1.000E+2 WL1 (nm) \$300.00 loaded definition file: Continue	V2(V) € 1.5000	of points after Voc after Voc	0.0200 increment (V) 0.0200 increment (V) 5 points per decade 10.00 increment (nm) Set Problem Save all simulations
F → ↓ C - ↓ C - ↓ F C-f F QE (IPCE) Set problem Calculate: single shot Calculate: batch	V1 (V) ⊈0.0000 V1 (V) ⊈0.8000 f1 (Hz) ⊈1.000E-2 WL1 (nm) ≇300.00 Ioaded definition file: Continue Batch set-up	V2(V) € 1.5000 V2(V) € 0.8000 2(Hz) € 1.000E+6 WU2(mm) € 200.00 Stop Results of ca EB G,R AC I-V	of points after Voc after Voc	0.0200 increment (V) 0.0200 increment (V) 5 points per decade 10.00 increment (nm) Set Problem Save all simulations Clear all simulations
F FV C-V C-F F QE (IPCE) Set problem Calculate: single shot Calculate: batch Calculate: recorder	V1 (V) \$0.0000 V1 (V) \$0.8000 f1 (H2) \$1.000E+2 WL1 (nm) \$300.00 loaded definition file: Batch set-up Record set-up	V2(V) € 15000 V2(V) € 0.8000 I2(Hz) € 1000E+6 WL2(mm) € 2d0.00 Stop Results of ca EB G,R AC IV Recorder	of points after Voc after Voc	0.0200 increment (V) 0.0200 increment (V) 5 points per decade 10.00 increment (nm) Set Problem Save all simulations Clear all simulations SCAPS info
F I+V C-V C C-F F QE (IPCE) Set problem Calculate: single shot Calculate: batch Calculate: recorder Calculate: curve fitting	V1 (V) \$ 0.0000 V1 (V) \$ 0.8000 f1 (H2) \$ 1.000E+2 WL1 (nm) \$ 300.00 I loaded definition file: Batch set-up Record set-up Curve fitset-up	V2(V) € 15000 V2(V) V2(V) € 0.8000 I2(H2) € 1000E+6 WL2(mm) € 200.00 Stop Results of ca EB G,R AC I-V Recorder Curvefitting	after Voc of points after Voc a 76 a a 81 a a 21 a a 171 a Problem file: new problem Idcutations C-V C-f QE results g results	0.0200 increment (V) 0.0200 increment (V) 5 points per decade 10.00 increment (nm) Set Problem Save all simulations Clear all simulations SCAPS info

Figure 5.12 Screenshot of the setting working condition

Step 3: Click on the Script set-up button, a window will pop up, click on the load button and select the script file you want to upload, and click on OK.

SCAPS 3.3.10 S	Script Editor Pane				
CAPS script (new	line with ENTER)			Final T	endem Connection.scri
SCAPS script lear all ad definitionfile C alculate singlesh jet iv xy // for top c jet characteristics et scriptvariable.y nath scalarabs yy r show scriptvarial bad definitionfile C alculate singlesh jet iv zu // for botto jet characteristics set scriptvariable.y	GaAs Topcell.def// ot .ell: v is stored in xve .jsc yvalue // jsc is s .yvalue yvector[0] // the first calculate bles Ge Bottom Solar cel ot .m cell: v is stored ir .jsc uvalue // jsc is s .vvalue 0.002 // start	or your deffile of the top actor, i in yvector tored in yvalue the first calculated J valu d  J  value is in y I.def // or your def file of t uvector, i in vvector tored in uvalue varying Jtandem from Js	cell (need to be in the s e is in y he top cell (need to be c(top) + this increment	in the scaps/def	Save Load Cancel OK
Insert Script part	ts: accept first propo	sed with F3 or select by	double-clicking below		
Command	Argument 1	Argument 2	Argument 3	Argument 4	Value

Figure 5.13 Process of loading tandem script

Step 4: Finally click on the Execute script button and get a result.

SCAPS 3.3.10 Action Panel							- 🗆 ×			
Working point           Temperature (K)           Voltage (V)           Voltage (V)           Frequency (Hz)           1.000E+6           Number of points	Series residence in the series	stance s Rs Ohm.cm S/cm	Shunt resis yer no ^2 Rsh ∎1. ^2 Gsh ∎1.	tance	Action lis     Load Action     Save Action	List	All SCAPS settings Load all settings Save all settings			
Illumination: Dark Light Specify illumination spectrum, then calculate G(x) Directly specify G(x)										
Analytical model for spectrum Spectrum file name: illumin Select spectrum file Spectrum cut off ?	AM1_5 Short wavel. (nm) \$400 Long wavel. (nm) \$400	ted from right G 1 sun.spe 0.0	Incider light pow sun or lamp 10 after cut-off 10	t (or bias) er (W/m2) 100.00	G(x) model Ideal Light Cur Transmission o	Constant ger rent in G(x) (m/ f attenuation fi	G(x) from file neration G			
Neutral Density 🚔 0.0000	Transmission (%) 🚔 100	.000	after ND 10	00.00	Ideal Light Cu	rrent in cell (m/	A/cm2) 0.0000			
Action Pau	se at each step	V2 (V)	<b>1.5000</b>	Stop after	of points Voc 276	€ 0.0200	increment (V)			
□ C-V	V1 (V) 🖨 -0.8000	V2 (V)	€ 0.8000		<b>\$</b> 81	\$ 0.0200	increment (V)			
C-f	f1 (Hz) 🚔 1.000E+2	f2 (Hz)	\$ 1.000E+6	J .	21	\$5	points per decade			
CE (IPCE)	WL1 (nm) 🖨 300.00	WL2 (nm)	2000.00	J	\$ 171	<b>10.00</b>	increment (nm)			
Set problem	loaded definition file:			Prob	olem file: new proble	m Set Prot	blem			
Calculate: single shot	Continue	Stop Results of calculation			ations	Sa	ave all simulations			
Calculate: batch	Batch set-up	EB G,R AC I-V C-V C-F QE Clear all simulations								
Calculate: recorder	Record set-up	Recorder results					SCAPS info			
Calculate: curve fitting	Curve fit set-up	Curvefitting results								
Execute script	Script set-up		Script graph	is S	cript variables		Quit			

Figure 5.14 Script Execution

#### 5.8 Scaps-1D Script used for simulation of multijunction solar cell

The script that is used for the simulation of multijunction solar cell is provided below

load definitionfile GaAs Topcell.def //top cell file stored in definition folder with the file extinction type(.def) calculate singleshot // this code will simulate individually top cell get iv ab // extracting j-v curve of top cell and placing i in b vector and v in a vector get characteristics.jsc bvalue // store value of J\_sc corresponding to top cell in b vector. set scriptvariable.bvalue yvector[0] // stoting J\_sc in b-vector math scalarabs bb load definitionfile Ge Bottom Solar cell.def // bottom cell file stored in definition folder with the file extinction type(.def) calculate singleshot// this code will simulate individually bottom cell get iv cd // extracting j-v curve of bottom cell and placing i in d vector and v in c vector

get characteristics.jsc uvalue

set scriptvariable.vvalue 0.003 // Begin changing Jtandem from
Jsc(top) + this increase (in mA/cm2)

math scalarsubtract vvy // The beginning value for Jtandem

set scriptvariable.wvalue 0 // Jtandem's stop value

set scriptvariable.bvalue vvector[loopcounter] math interpolate xXyY //Determine the bottom cell's voltage at this junction (via interpolation); set its inzuvalue set scriptvariable.uvalue vvector[loopcounter] math interpolate zZuU // Perform the series connection: When the top and bottom cell voltages are added, the result is in xvalue. math scalaradd xxz set scriptvariable.wvector[loopcounter] xvalue // and enter this value (x) in the vector w loop stop // Give the vectors appropriate names, then plot them set scriptvariable.xname Vtop set scriptvariable.yname Jtop set scriptvariable.zname Vbottom set scriptvariable.uname Jbottom set scriptvariable.wname Vtandem set scriptvariable.vname Jtandem show scriptvariables plot draw wv // plot j-v of tandem cell plot draw xy // plot j-v of top sub cell plot draw zu // plot j-v of bottom sub cell // obtaining the tandem's efficiency metrics and placing it in the scalars x vector, y vector, z vector, u vector, v vector, w vector math characteristics.voc xwv math characteristics.jsc ywv math characteristics.ff zwv math characteristics.eta uwv math characteristics.vmpp vwv math characteristics.jmpp wwv show scriptvariables

### 5.9 Result of simulation



J-V curves of individual top and bottom cells are illustrated below.

Figure 5.15 J-V curve of the top (GaAs) solar cell (b) J-V curve of the bottom (Ge) solar cell (c) J-V curve of the tandem Cell

The J-V curve of the resultant two-junction tandem cell is illustrated in Figure 5.15(c) by the plot in red colour. According to our assumption ideality of tunnel junction, the short circuit current density regarding to multijunction solar cell is equal to the current density of the cell that produces the lowest short circuit current density. Subcells were connected in series so the resultant  $V_{OC}$  will the sum of individual  $V_{OC}$  produced by the subcell. A screenshot of extracted external parameters is depicted in Figure 5.16.

💽 SCAPS 3.3.10 Sc	—	$\Box$ $\times$							
General SCAPS script variables									
mode 0 filename: defaultfilena loopcounter 99 max. nr. of iterations1 looperror 1.000000e- maxerror 1.000000e-	ame 00 ⊦30 03				ى ئى				
uvalue 2.8090E+1	vvalue 1.1176E+0	wvalue 2.5134E+1	xvalue 1.2705E+0	yvalue 2.6008E+1	zvalue 8.5007E+1				
Jbottom 0-2.85136e+01 4 1-2.85136e+01 3 2-2.85069e+01 3-2.84970e+01 4-2.84296e+01 6-2.83299e+01 7-2.81143e+01 8-2.76478e+01 9-2.66393e+01 10-2.44613e+01 11-1.97693e+01	Jtandem (mA/cm2) 0-2.59114e-01 1-2.56497e+01 3-2.51262e+01 4-2.48645e+01 5-2.46028e+01 6-2.43410e+01 7-2.40793e+01 8-2.38176e+01 9-2.35558e+01 10-2.32941e+01 11-2.30324e+01	Vtandem (V) 0 2.90522e-01 4 1 1.08060e+00 2 1 1.0368e+00 3 1.11793e+00 4 1.12811e+00 5 1.13828e+00 6 1.14401e+00 7 1.14882e+00 8 1.15363e+00 9 1.15844e+00 10 1.16326e+00 11 1.16703e+00 3	Vtop (V) 0 0.00000e+00 4 1 2.00000e-02 3 3 6.00000e-02 4 5 1.00000e-02 5 1 0.00000e-01 6 1 2.0000e-01 8 1 6.0000e-01 8 1 0.20000e-01 10 2.0000e-01 11 2.00000e-01 11 2.0000e-01 11 2.00000e-01 11 2.0000e-01 11 2.0000e-01 11 2.00000e-01 11 2.0000e-01 11 2.00000e-01 11 2.00000000000000000000000000000000	Jtop (mA/cm2) 0-2.59134e+01 1-2.59126e+01 3-2.59126e+01 3-2.59126e+01 5-2.59115e+01 6-2.59111e+01 7-2.59107e+01 8-2.59103e+01 9-2.59099e+01 10-2.59095e+01 11-2.59090e+01	Vbottom (V) 0 0.00000e+00 4 1 2.00000e-02 2 4.00000e-02 3 6.00000e-02 4 8.00000e-02 5 1.00000e-01 6 1.20000e-01 7 1.40000e-01 9 1.80000e-01 10 2.00000e-01 11 2.20000e-01				
Stop script execution		Contir	nue	Save script variables					

Figure 5.16 Screenshot of the extracted external parameters

here the different vector value holds different external parameters such as

x vector—holds the  $V_{OC}$  of the tandem solar cell.

y vector—holds the  $J_{SC}$  of the tandem solar cell.

z vector—holds the FF of the tandem solar cell.

u vector-holds PEC of the tandem solar cell.

v vector-holds the maximum operating voltage.

w vector-hold maximum operating current density.

The  $V_{OC}$  of 1.27 volts has been obtained with a  $J_{SC}$  of 26.00mA/cm<sup>2</sup> and a FF of 85% with a PCE of 28.10%.

Now will see the spectral utilization of a multijunction solar cell illustrated in Figure 5.17, red curve reflects the spectral utilization of high band gap material(GaAs top cell) which uses the lower wavelength part of the spectrum and on the other side blue curve reflects the spectral utilization of low band gap material(Ge bottom cell) which uses higher wavelength part much more efficiently, hence by using two junctions solar cell we are able to exploit much part of the solar spectrum.



Figure 5.17 QE of the two-junction tandem solar cell

## Chapter 6 -Conclusion and Feature Scope

### 6.1 Conclusion

In this, I set out to investigate the loss and the generation mechanisms occurring within the solar cell, the domain of the study of the loss mechanism is concise to variation in defect concentration, and finally, by using some mathematical empirical relations we practices to connect Urbach energy with one of the external parameter the Open-circuit voltage. To utilize the full potential of the fabricated device, a generation mechanism has also been explored, where we optimize the single junction solar cell by optimizing various parameters independently which are ETL thickness, HTL thickness, absorber material thickness, and the acceptor doping density, to an extreme level so that finally we have a best fine-tuned device. As far as single junction solar cells are concerned there is a maximum theoretical limit up to which the device can transform light energy into electrical energy so, called the Shockley Quiesser limit, which the band gap of the material can determine, this upper limit is due to restriction in the spectral utilization by the single junction solar cells. The way to overcome this limit is to remove the restriction of the spectral utilization which can be achieved by using multi-junction solar cells. The major findings of the research work reported in this thesis are sequentially summarised.

### 6.1.1 Major findings related to loss mechanism

- ✓ Open-circuit voltage of the solar cells, depends on the splitting in the quasi-fermi level which is further limited by the recombination mechanism.
- ✓ The greater the splitting between quasi-Fermi levels, the higher the open-circuit voltage. This results in better utilization of the band gap of the absorber material.
- ✓ Higher recombination leads to a lower open-circuit voltage, due to less splitting in quasi-fermi level. As a result, the band gap is not utilized efficiently.
- ✓ One-to-one correspondence between Open-circuit voltage( $V_{OC}$ ) and Urbach energy( $E_U$ ).
- ✓ Hence, Urbach energy becomes an important diagnostic parameter in studying the loss mechanism originating due to structural disorder.

#### 6.1.2 Major findings related to the generation mechanism

- ✓ While optimizing the device, it has been figured out that ETL thickness should be kept as thin as possible.
- ✓ It is crucial to note that the thickness of the HTL does not significantly affect the performance of the device.
- ✓ Absorber thickness should be optimized to the limit until the generation mechanisms are dominant as compared to the loss mechanism.
- ✓ Absorber material should be doped to reduce SRH recombination losses and up to some extent it also modifies the band alignment which leads to the changes in splitting in quasi-fermi levels.
- ✓ Before optimizing the device, the efficiency we achieved was around 16.47% and after finetuning the device, the efficiency increased to around 22.49%.
- ✓ In the case of the multijunction solar cell, a simulation is performed by keeping two junctions one over the other, where GaAs work as the cell and Ge acts as the bottom cell, the PCE of the device is 28.10%. Which is much higher than the PCE achieved by the individual top cell (GaAs-23.24%) and bottom cell (Ge-7.36%).

## 6.2 Feature Scope

### 6.2.1 Capacitance-Voltage(C-V) analysis

Using capacitance-voltage analysis one predicts important information about the structure of the p-n junction, such as the height of the potential barrier.

Two factors are responsible for the capacitance in p-n junction the first one is Junction capacitance (dominant under reverse bias) and the second is diffusion capacitance (dominant under forward bias).

In the context of solar cell diffusion-capacitance provides very useful information on whether the device that we have fabricated and how efficiently the transportation of the charge carrier will take place.

### 6.2.2 Capacitance-frequency(C-f) analysis/admittance spectroscopy

Admittance spectroscopy allows us to accurately characterize the energy distribution of the defect within the absorption layer of a solar cell.

By analyzing the c-f characteristics of the device, we can extract information about the defect activation energy and concentration.

Changes in the defect properties before and after a process like annealing can be studied using admittance spectroscopy.

# Appindix1

S.No.	ETL	eta(%)	V <sub>OC</sub> (volt)	$J_{SC}(mA/cm^2)$	FF(%)
	Thickness(inµm)				
1	0.03	21.16097	1.00881	25.73495	81.50847
2	0.05	20.17124	1.00771	25.12009	79.68512
3	0.07	18.69283	1.00547	23.78188	78.17318
4	0.09	17.17894	1.00302	22.04043	77.70784
5	0.11	15.80357	1.00062	20.31811	77.73254
6	0.13	14.5887	0.99805	18.76355	77.90244
7	0.15	13.51808	0.99553	17.38882	78.08879
8	0.17	12.56233	0.99318	16.17402	78.20316
9	0.19	11.72342	0.99097	15.09701	78.36185
10	0.21	10.97707	0.98888	14.13878	78.51088
11	0.25	9.71567	0.98506	12.51851	78.78751
12	0.3	8.48029	0.98085	10.93073	79.09708
13	0.35	7.52798	0.97676	9.70638	79.40219
14	0.4	6.77993	0.97318	8.75135	79.60844
15	0.45	6.19462	0.97012	7.99807	79.83724
16	0.5	5.72813	0.9675	7.39755	80.03402

## Data related to the ETL

## Data related to the doping concentration of the absorber material

S.No.	Absorber Acceptor	eta(%)	$V_{OC}(volt)$	$J_{SC}(mA/cm^2)$	<i>FF</i> (%)
	concentration(cm <sup>2</sup> -3)				
1	0	16.43692	1.0014	21.14125	77.63977
2	1E+10	16.43692	1.0014	21.14125	77.63977
3	1E+11	16.43695	1.0014	21.14127	77.63983
4	1E+12	16.43725	1.0014	21.14146	77.64027
5	1E+13	16.44036	1.00144	21.14336	77.64509
6	1E+14	16.47089	1.00181	21.16235	77.69044
7	1E+15	16.74418	1.00613	21.35226	77.94133
8	1E+16	17.93078	1.04298	22.91253	75.03248
9	1E+17	18.24425	1.09429	22.78748	73.16373
10	1E+18	16.06491	1.13299	19.56181	72.48444

## Appindix2

#### Exponential decay of the excess charge carriers

The diffusion equation for the electron is given by[3]

$$\frac{\partial \delta_n}{\partial t} = D_n \frac{\partial^2 \delta_n}{\partial x^2} - \frac{\delta_n}{\tau_n} \qquad \dots 1$$

At steady state condition

$$\frac{\partial \delta_n}{\partial t} = 0 \qquad \dots 2$$

Equation 1 will be simplified to

$$D_n \frac{\partial^2 \delta_n}{\partial x^2} = \frac{\delta_n}{\tau_n}$$
$$\frac{\partial^2 \delta_n}{\partial x^2} = \frac{\delta_n}{D_n \tau_n} \qquad \dots 3$$

We know that the relation between diffusion coefficient, lifetime, and diffusion length is given by

$$L_n = \sqrt{D_n \tau_n} \qquad \dots 4$$

Putting this value in Equation 3 we get

$$\frac{\partial^2 \delta_n}{\partial x^2} = \frac{\delta_n}{L_n^2} \qquad \dots 5$$

Let us assume that excess electrons are somehow injected into a semi-infinite semiconductor bar at x=0, and steady-state electron injection maintains a constant excess hole concentration at the injection point,

$$\delta_n(x=0) = \Delta n \qquad \dots 6$$

Solving, second-order linear homogenous differential equation 5. We get,

$$\delta_n(x) = Ae^{\binom{-x}{L_n}} + Be^{\binom{x}{L_n}} \qquad \dots^7$$

Subjecting boundary condition, at  $x \to \infty$ ,  $\delta_n(x) = 0$ 

$$\Rightarrow B = 0$$

Hence, equation 7 will become

$$\delta_n(x) = A e^{\left(-x/L_n\right)} \qquad \dots 8$$

Again subjecting boundary condition, at x = 0,  $\delta_n(x) = \Delta n$ 

$$\Rightarrow A = \Delta n$$

Now, equation 8 will become,

$$\delta_n(x) = \Delta n e^{\left(-x/L_n\right)} \qquad \dots 9$$

Equation 9, gives the significance of the exponential decay of the injected excess carrier electrons.

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