Efficiency Analysis and Optimization of Light Trapping in Amorphous Silicon Heterojunction Solar Cell with Lumerical FDTD/DEVICE

By

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“Efficiency Analysis and Optimization of Light Trapping in Amorphous Silicon
Heterojunction Solar Cell with Lumerical FDTD/DEVICE”

by Muhammad Riaz

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ABSTRACT
Title: Efficiency Analysis and Optimization of Light Trapping in Amorphous Silicon Heterojunction Solar Cell with Lumerical FDTD/DEVICE
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This study investigated the two-dimensional computer analysis of a tandem solar cell: c-Si/a-Si:H/μc-SiGe, with Lumerical FDTD/DEVICE 4.6. Optical characterization was performed in FDTD and then the total generation rate was transported into DEVICE for electrical characterization. Electrical characterization of the solar cell was carried out in DEVICE. In the first stage, a single junction solar cell was studied with both a-Si and μc-SiGe, respectively, as its absorbing layers. The thickness for both layers was kept the same. For the a-Si absorbing layer $J_{sc} = 10.959 \text{ mA/cm}^2$, $V_{oc} = 696.97 \text{ mV}$, $FF = 78.985\%$, and $\eta = 6.033\%$ were achieved. The efficiency for the μc-SiGe absorbing layer was improved up to $\eta = 7.0667$. In the second stage, with the implementing tandem design for the thin film solar cell as c-Si/a-Si:H/μc-SiGe; the $J_{sc} = 16.4136 \text{ mA/cm}^2$; $V_{oc} = 732.323 \text{ mV}$; $FF = 81.9017\%$; and $\eta = 9.84462\%$ were recorded. Moreover, three different light trapping techniques were compared with the efficiencies of planner solar cell and with anti-light reflecting coatings (TIO$_2$ and SI$_3$N$_4$). The efficiency is optimized with Checkerboard Light Trapping Design (QPEC), as $\eta = 12.397\%$. The increase in efficiency is 20.5% as compared to the planer solar cell, 17.2% as compared to the Pyramidal Technique, and 15.42% as compared to ITO and SI$_3$N$_4$. In the QPEC technique, the percent increase in efficiency is 9.2% as compared to the planer solar cell and 3.3% increase as compared to ITO and SI$_3$N$_4$. With Pyramidal Design, light trapping is increased to 4.1% as compared to the planer solar cell and 2.17% reduced as compared to ITO and SI$_3$N$_4$. The efficiencies for both ITO (TIO$_2$) and SI$_3$N$_4$ antireflection coatings are noticed to be same as $\eta = 10.4855\%$. By insertion of a buffer layer at the second interface from the top, the efficacy is improved up to $\eta = 13.065\%$. 
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DEDICATION

I dedicate this accomplishment to my parents: my father Raja Mir Aman Khan and my mother Ashraf Bibi; my eldest brother Raja Sartaj Alam and my wife Hafsa. You have always shown your unconditional love, care, and support that can never be compensated for by anything in the world.
Chapter 1

Introduction
INTRODUCTION

Consuming energy by ensuring conservation of the environment is the most challenging task for sustainable development. This can only be attained by emphasizing the development of the renewable energy industry and by improving its economic value. One of the best sources of energy is sunlight. There is a great potential to have sunlight contribute to renewable energy, especially solar energy, which makes up less than one percent of the total energy produced from renewable sources at present (Haque, Quddus, Ferdaous, & Hoque, 2013). This study is to assess the most economical solar technologies that have the potential to become a larger component of the future energy portfolio. Up to now, the most economical technology is Silicon (Si) based technology. Si has a lower control on intrinsic charge carrier generation and has low performance at high temperature. It also has less endurance to caustic harsh environment. Regardless of these disadvantages, Si is still an option for the electronic and photovoltaic (PV) industry. Si technology is very cost effective and environmentally friendly compared to other technologies and materials. Despite its limitations, for example, its switching frequency, efficiency, and reliability, Si is still a promising cost effect source in abundance (Nawaz, 2011). Silicon is available in pure crystalline (c-Si), poly crystalline (pc-Si), and in amorphous (a-Si) forms. Amorphous silicon (a-Si) is considered the cheapest source in PV designing. Researchers are still taking a pragmatic approach with a wide range of options to improve its efficiency by using a-Si with its alloys. The high potential of this technology has been recently demonstrated by Sanyo reaching 22.80% cell efficiency in the lab (Mishima, Taguchi, Sakata, & Maruyama, 2011) and 15.00% in a commercial module (Grigovici, Croitoru, Marina, & Natasi, 1968).

For this study, an amorphous silicon tandem (hetero-junction) solar cell is designed and investigated with Lumerical FDTD/DEVICE and AFORS–HET. With Lumerical FDTD/DEVICE, an amorphous silicon tandem solar cell, c-Si/a-Si:H/μc-SiGe, is investigated and its optical and electrical characterization is carried out. The optical characterization is performed in FDTD and then the total generation rate is
transported into DEVICE for electrical characterization. The Electrical characterization of the solar cell is carried out in DEVICE. The maximum efficiency for a single junction thin film solar cell c-Si/µc-SiGe and tandem solar cell c-Si/a-Si:H/µc-SiGe is achieved. Three different light soaking designs for thin film solar cell are designed and their efficiency is optimized. The light trapping techniques are investigated and compared. The checkerboard (QPEC), pyramidal structure, and quarter pyramid in empty checker light capturing techniques are designed. The efficiencies of these techniques are compared with the efficiency of a planner (without textured) solar cell and with anti-reflecting (AR) layers of ITO (TIO₂) and Si₃N₄.

In AFORS–HET, a p-i-n tandem hetero-junction solar cell, with top p⁺ and the bottom n⁺ layers, each 5nm thick, is designed with doping concentrations of Na = 3x 10¹⁸ cm⁻³ and Nd = 8x 10¹⁸ cm⁻³ respectively. The mid-intrinsic region of this hetero-junction solar cell is divided into amorphous hydrogenated silicon (a-Si:H), 110nm thick and amorphous silicon alloyed Germanium (a-SiGe:H) with a thickness of 80nm. The top absorbing layer is an a-Si:H layer with a graded band gap from 1.75eV to 1.65eV. The second absorbing layer is a-SiGe:H with a fixed band gap 1.55 eV. A thin film of indium tin oxide (ITO) 80nm can serve as an anti-reflector. A 10nm wide band gap (1.85eV) thin intrinsic a-SiC is used as a window for the a-Si:H layer. This layer helps to reduce the interface recombination and improves the interface quality with better surface passivation. The pure intrinsic silicon, a-Si(i) 10nm thick, is used as a buffer layer between the absorbing layers. Ag is used as the top and bottom contact with a thickness of 20.00nm. The built-in field across this region is used for separation of electron hole pairs. The difference in band gap energies of the upper layer a-Si:H with Eg = 1.75 to 1.65 eV to the lower layer a-SiGe with Eg = 1.7eV will allow absorption of a broadened range spectrum and hence the efficiency of the device is predicted to increase. By varying the width of the intrinsic layer, the efficiency (η), open circuit voltage (Voc), and fill-factor (FF) of the cell is improved. The known parameter band gap and mobility of the carriers is kept unchanged. Finally, the device is modeled to
optimize the efficiency by using AFORS-HET (Automate for simulation of Heterostructures) software 2.4.1.

1.1 Amorphous Silicon (a-Si) and a-Si Doped Ge

Silicon is the most widely used material in the electronics industry due to its low cost and availability. It is the eighth most common element in the universe by mass, but it is very rarely available as a pure free element in nature. It is available in the form of dust, sand, and silicon dioxide (silica). On earth, silicon is the second most abundant element after oxygen and exists in the earth’s crust about 28% by mass. It is categorized by quality, which is a trade off with its efficiency and cost. Processed crystalline silicon wafers are more costly; they make up 40 to 50% of the cost of a finished module (Shah, Torres, Tscharner, Wyrsch, & Keppner, 1999).

The basic properties of Si are shown and compared with GaAa, GaN and SiC in Table 1.1 and the basic material properties of amorphous silicon are shown in Table 1.2.

Table 1.1

Comparing Properties of Silicon with Other Materials Taken at 300K

<table>
<thead>
<tr>
<th>Properties</th>
<th>Si</th>
<th>3C-SiC</th>
<th>GaN</th>
<th>GaAs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eg (eV)</td>
<td>1.12</td>
<td>2.20</td>
<td>3.39</td>
<td>1.42</td>
</tr>
<tr>
<td>ni (cm$^{-3}$) at 300K</td>
<td>1.45x10$^{10}$</td>
<td>6.9</td>
<td>1.6x10$^{-10}$</td>
<td>1.8x10$^6$</td>
</tr>
<tr>
<td>εr</td>
<td>11.7</td>
<td>9.72</td>
<td>9.00</td>
<td>13.1</td>
</tr>
<tr>
<td>μn (cm2/Vs)</td>
<td>1400</td>
<td>900</td>
<td>900</td>
<td>6500</td>
</tr>
<tr>
<td>μp (cm2/Vs)</td>
<td>471</td>
<td>40</td>
<td>850</td>
<td>320</td>
</tr>
<tr>
<td>Vsat (107 cm /s)</td>
<td>1.0</td>
<td>2.0</td>
<td>2.5</td>
<td>1.2</td>
</tr>
<tr>
<td>Ecrit (MV/cm)</td>
<td>0.3</td>
<td>1.2</td>
<td>3.3</td>
<td></td>
</tr>
<tr>
<td>κ (W/cm .C)</td>
<td>1.5</td>
<td>4.5</td>
<td>1.3</td>
<td>0.5</td>
</tr>
</tbody>
</table>

(Neudeck, 1995; Tairov & Tsvetkov, 1978; Van Daal, Knippenberg, & Wasscher, 1963)
The microcrystalline silicon and amorphous silicon are relatively cost effective but have low efficiency. Amorphous silicon is used in thin films. It not only has a lower investment cost, but it also shows good characteristics in absorbing certain

Table 1.2

*Material Properties of Hydrogenated Amorphous Silicon (aSi:H)*

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Band gap (eV)</td>
<td>1.4 - 1.9</td>
</tr>
<tr>
<td>Hydrogen content (%), typical</td>
<td>10 – 30</td>
</tr>
<tr>
<td>Density (g/cm³) for two hydrogen concentrations</td>
<td>2, 20 at 10% hydrogen content</td>
</tr>
<tr>
<td>Dielectric constant for two hydrogen concentrations</td>
<td>14 at ( N_H = 5 \times 10^{21} \text{ cm}^{-3} )</td>
</tr>
<tr>
<td></td>
<td>16 at ( N_H = 17 \times 10^{21} \text{ cm}^{-3} )</td>
</tr>
<tr>
<td>Intrinsic specific resistivity (Ω cm)</td>
<td>2 x ( 10^{10} ) at room temp</td>
</tr>
<tr>
<td>Maximum specific conductivity after doping (Ω cm)</td>
<td>( 10^{-2} ) at room temp</td>
</tr>
<tr>
<td>Effective states density at the conduction band edge, ( N_c ) (cm(^{-3}))</td>
<td>( 4.5 \times 10^{21} )</td>
</tr>
<tr>
<td>Effective states density at the valence band edge, ( N_v ) (cm(^{-3}))</td>
<td>( 6.5 \times 10^{21} )</td>
</tr>
<tr>
<td>State density at mid gap (cm(^{-3}))</td>
<td>( 10^{17} - 10^{18} )</td>
</tr>
<tr>
<td>Recombination lifetime (s)</td>
<td>( 10^{-9} - 10^{-2} )</td>
</tr>
<tr>
<td>Drift and mobility (cm(^2)/Vs) electron/holes</td>
<td>1 / 0.01</td>
</tr>
</tbody>
</table>

(Seale, 1998; Street, 2005)

Radiation spectrums. The disadvantage is its significant degradation of up to 15 to 35% (Shah et al., 1999) when exposed to light for a long time. However, with doping Ge into a-Si, the degradation process can be slowed down by accommodation of dangling bonds. This also changes the energy band gap of the material. Silicon and amorphous silicon can be easily deposited on a large area to make solar cell.
1.2 History and Structure of Si

Silicon is a tetravalent metalloid, having atomic number 14 with symbol Si. It belongs to group IV of the periodic table. It has a diamond cubic structure. It is not a reactive element but it is more reactive than germanium. It has a larger band gap (1.1eV) than germanium and has a better ability to operate at higher temperatures. There is controversy about the exact date of discovery of silicon, but it is known that it was first prepared and characterized in pure form in 1823 (Seitz & Einspruch, 1998). In the early 1900s, before integrated circuits and silicon chips, computers and radios were made with vacuum tubes and these tubes were used to conduct, modulate, and amplify electrical signals. In the search for the replacement of these vacuum tubes, scientists began studying the electrical properties of semiconductors and invented the first semiconductor-based transistor in 1947 in Bell Lab. The first commercial transistor was introduced in 1957. In 1958, Kilby demonstrated the first working IC.

![Figure 5.1](image)

**Figure 5.1** a) Si atomic configuration, b) position in periodic table and c) physical structure.

In 2000 Kilby won the Nobel Prize in Physics for his part in this invention. After 1960, the manufacturing of semiconductor (Si and Ge) devices had spread to the rest of the world. Silicon wafers are made of pure silicon that is grown into
mono-crystalline cylindrical ingots up to 300mm in diameter and are used as substrates for microelectronic devices. The modern ICs are made of silicon wafers through the process called stepping. These silicon wafers are moved in many steps (doping, ion implantation, etching, and deposition) under a mask in order to expose them to UV-light (photolithography and patterning).

The investigation about amorphous silicon, especially working on a hetero-junction between amorphous silicon and crystalline silicon, started since last 45 years. The first hetero-junction reported by Grigorivici (Grigorovici et al., 1968) was a-Si/c-Si hetero-junction. It was designed by evaporation of amorphous non-hydrogenated silicon at room temperature on top of p or n type crystalline silicon with a different resistive method and annealing of the deposited film at different temperature. Later on with the continuing research on Schottky diodes, Brodsky had given a detailed analysis of the current transport mechanism in intrinsic amorphous silicon on crystalline silicon hetero-junction. With time, the amorphous silicon emerged as the most cost-effective material in photovoltaic applications and was used as n-type a-Si:H on a p-type polycrystalline silicon a-Si:H/c-Si hetero-junction solar cell. In 1992, Sanyo presented a new type of hetero-junction solar cell, which was named the HIT Solar cell; it used the p-type amorphous silicon on n-type crystalline silicon with a very thin intrinsic interface layer (Tanaka, Taguchi, & Matsuyama, 1992).

1.3 Energy Band Diagram

An energy band diagram is a model of the electron and holes available for the current flow in the material. This model defines the type of the material, it is either an insulator, conductor, intrinsic semiconductor, or a doped semiconductor (Pierret, 1996). The valance band is the lowest allowed energy state where electrons are not free to conduct. The electrons in the valance band are part of the atomic bonds. The conduction band is the band of allowed energy states where electrons are freed from atomic bonds and are free to contribute to current flow. Electrons tend to settle at the lowest allowed energy in the valance band. Valance
electrons, when they gain energy equal to the band gap \((E_g = E_c - E_v)\), then they move to the conduction band electrons. Different materials have a different band gap energy \(E_g\); for example Si has \(E_g = 1.12\) eV, Ge has \(E_g = 0.67\) eV and SiO\(_2\) has \(E_g = 8\) eV. The important concept of the energy band model is elaborated in Figure 1.2.

![Energy band diagram](image)

**Figure 1.6** Energy band diagram for three different type of material (Floyd & Buchla, 2002)

The fermi level \(E_F\) defines the probability that an energy state will be filled by an electron and can be defined by using the Fermi-Dirac distribution function as given in the following:

\[
f(E) = \frac{1}{1 - e^{(E-E_F)/kT}}
\]

where \(f(E)\) is the probability that an energy state at \(E\) is filled, \(E_F\) is the Fermi level, \(k\) is Boltzmann’s constant \((8.62 \times 10^{-5}\) eV/K), and \(T\) is the temperature in Kelvin. \(E_F\) is located at \(E_g/2\) or halfway between the band gap. At a temperature of \(0\) K, the probability of filling an energy state located above \(E_F\) is zero. For a temperature greater than zero kelvin, the probability of occupying an energy state at \(E_F\) is one half; most energy states will be filled for energies at \(E_F - 3kT\) or below, while most energies will be empty for energies at \(E_F + 3kT\) and above (Pierret, 1996).
1.4 Photon Absorption and Carrier Generation in Direct and Indirect Band Gap

The band gap diagram of silicon is shown in Figure 1.4 where it is clear that any photon with energy greater than 1.1eV (in the range of 1.1eV to 3.4eV) can be observed through an electronic transition. The excitation of an electron from valance band to an empty state in the conduction band or to a defect state, which requires momentum from a photon, makes absorption less likely than the direct band transition. Since the silicon has a band gap of 1.12eV, which is in the near infrared region, crystalline silicon has poor absorption efficiency for the visible and ultraviolet spectrum. Therefore, it must have a thick wafer (about one hundred to three hundred micron) for efficient photon absorption. The amorphous silicon has an advantage and better efficiency in the form of thin film for optical absorption. The a-Si is a good thin film photovoltaic material, having a band gap of 1.48ev, and the absorption increases by impurity scattering.
1.5 Heterojunction Technique

The heterojunction technique is used in third generation tandem solar cells. A tandem cell is made of multiple junctions with different band-gap energies. When light with a broadened spectrum passes through multiple junctions, each junction can absorb a particular energy of photon and tune to a particular spectrum according to the band gap energy. Overall, it increases the total absorption and efficiency of a cell by the spectrum splitting mechanism. This method also reduces the energy loss by the thermalization of hot electrons generated by the absorption of photons by indirect band gap transitions.

In this study, the amorphous silicon solar cell consists of two absorbing layers, a-Si:H and a-SiGe. The top layer is an intrinsic silicon hydrogenated layer with a graded band gap of 1.75eV to 1.65eV. The second layer, a-SiGe has a fixed bandgap of 1.55eV. There are other a-Si layers, which are inserted to enhance the performance of the heterojunction. There are some other materials with promising high efficiency but these materials are expensive and have difficulties in harvesting solar energy at a larger scale.
1.6 The Conversion of Solar to Electrical Energy

The basic theory behind the electric current generation by photovoltaic devices is the conversion of photon energy into electron hole pairs, where the incident photon must have energy equal to or greater than the band gap of the semiconductor material; otherwise, it will be transmitted through the material. These free photo or thermal generated carriers will be separated by an electric field and transported to the contact through the bulk.

There are two types of the semiconductors used in photovoltaic devices, organic and inorganic. In the organic material, the current is achieved with the help of an excitron (a combination of an electron and hole by cumbolic attraction force) dissociated across the energy gradient. The band gap is to be determined by the top occupied molecular orbital and the lowest unoccupied molecular orbital. The operations in an organic photovoltaic are fundamentally different from an inorganic photovoltaic, which is determined by the molecular orbits and is built of the summations of all atomic orbitals in the molecule. In inorganic semiconductors, such as Si, Ge, GaAs, and InGaAs, there must be a p n junction where the excess carriers are separated with the help of an electric field by reverse biasing. The efficiency of these devices is determined by the ability of the photo-generated minority carriers to reach the p-n junction before recombination with the majority carriers in the bulk of the material. Thus, the bulk properties often control the device efficiency.

1.7 Efficiency of Solar Cell

Efficiency of a solar cell is basically the percentage of solar energy converted into electrical energy or current. The factors affecting the efficiency of solar cell are wavelength of incident light, natural (bulk) resistance, temperature, reflection, and electric resistance. The conversion efficiency of a solar cell, \( \eta \) is given in the following (Haque et al., 2013):

\[
\eta = \frac{V_{oc} \cdot J_{sc} \cdot FF}{E} \times 100\%
\]
where

\( V_{oc} \) : Open-circuit voltage (in volt)

\( J_{sc} \) : Short-circuit current density (in A/cm\(^2\))

\( E \) : Solar irradiance on earth (in W/cm\(^2\))

\( FF \) : Fill Factor (defined in the next section)

Usually, efficiency is calculated with the AM 1.5G and \( E = 0.1 \) W/cm\(^2\).

1.8 Maximum Power Point

The output power is zero when the solar cell is in the short circuit or the open circuit condition. In between these two limits, when load resistance increases from zero to infinity on an irradiated solar cell, there will be a point where the solar cell can deliver maximum output power. This point for a load where the cell delivers maximum output power is called the maximum power point.

1.9 Fill Factor (\( FF \))

The fill factor is defined as the ratio of the actual maximum achievable power to the product of the open circuit voltage and short circuit current. This is one of the important parameters in defining overall performance of a solar cell. The commercial solar cells have a fill factor of usually more than 70\%. It is also defined as the maximum power point divided by the product of the short circuit current and open circuit voltage. It can be calculated by using the following equation (Haque et al., 2013):

\[
FF = \frac{V_{ocn} - \ln (V_{ocn} + 0.72)}{V_{ocn} + 1}
\]

where

\[
V_{ocn} = \left( \frac{q}{nkT} \right) V_{oc}
\]

here

\( V_{oc} \) : Open-circuit voltage (in volt)

\( n \) : Identity factor (Taken as 1)

\( q \) : Charge of an electron (in C)
1.10 Quantum Efficiency of Solar Cell (QE)

The quantum efficiency of a solar cell is the ratio of total collected charge carriers to the total number of incident photons of light. The quantum efficiency is defined as the function of either wavelength or energy, which is always affected by recombination and diffusion length. There are two types of quantum efficiency defined as follows (Green, Emery, Hishikawa, Warta, & Dunlop, 2015):

1. **External QE**: is related to the effect of all optical losses, including reflection and transmission. After measuring the total transmission and reflection of a solar cell, the external QE curve can be corrected to obtain the internal QE.

2. **Internal QE**: refers to the efficiency of a solar cell. It defines the total percentage of photons (after optical losses) converted to electric current when the cell is operating under the short circuit condition.

The quantum efficiency and the photo-generated current can be defined and related to the other parameters by giving these equations:

\[
\eta = \frac{R \nu}{q} = (1 - R) \exp(-aw) \left[1 - \frac{e^{-\alpha d}}{1 + \alpha L}\right], \quad I_{ph} = \frac{-q(1 - R)P_{ph}}{\hbar \nu} (1 - e^{-\alpha d})
\]

The quantum efficiency is based on the thickness of the intrinsic layer. The photocurrent depends on the both energy \( h \nu \) (Luque & Hegedus, 2011) and the thickness of the intrinsic layer ‘d’, theoretically.

1.11 Amorphous Silicon Photovoltaic Tandem Cell (a-Si:H + a-SiGe:H)

Usually the amorphous silicon is deposited on glass or on a plastic substrate at a low temperature as a thin film that absorbs the photons with a frequency equal to or above the band gap of silicon (1.1ev) (Street, 2005). The amorphous silicon is cheaper and only 1% is needed to fabricate a crystalline silicon photovoltaic (Zhu
et al., 2008) because it has the best absorption ability (one micro meter thickness has ninety percent absorption efficiency). Designing the a-Si junction is different from the normal p-n junction diode. It is designed in the form of p-i-n, which means that an intrinsic silicon material is sandwiched in between the two very heavily doped p and n type semiconductor materials. It contains three layers of silicon material (p+, i and n+). The heavily doped p+ and n+ layers are very thin to minimize the probability of a recombination of carriers during the transportation towards the contact. In case of the recombination in the p+ and n+ regions, the excess carriers generated by the photon will be wasted and they will not take part in the current. Hence, to maintain the electric field for the quick separation (Street, 2005) of the carriers, both the p+ and n+ regions must be heavily doped. The width of the intrinsic material is large (thick) enough as compared to the p and n regions to absorb a maximum number of photons; however, at the same time, the diffusion length of the carrier limits the total width of the intrinsic layer. The Intrinsic i layer is un-doped because the amorphous silicon is quite sensitive to defects and it may be aggravated further by added impurities. However, with doping of Ge, the band gap of the device can be varied along the thickness of the intrinsic layer.

The amorphous silicon material is susceptible to accommodating different types of atoms due to the defects such as induced by the dangling bonds. These are the major defects in the a-Si. The dangling bonds are the result of the broken weak bonds of hydrogen atoms in the a-Si through the passage of time. These defects cause deterioration in the probability of recombination and hence lower the quality of the material. If we are successful in reducing these defects and the dangling bonds, we may increase the efficiency of amorphous silicon. There are other techniques used to reduce these dangling bonds but we preferred to dope Ge in the a-Si to improve the quality of the thin film because of its easy availability. The doping mechanism also changes the lattice parameter and the band gap energy. We used these parameters to broaden the absorption spectrum of the material. The efficiency depends on the width of the intrinsic and extrinsic regions, which must be precisely calculated and assessed. In practice, the doping can be achieved in-
situ via deposition with saline gas (Luque & Hegedus, 2011). It is also possible to use cheaper methods for the amorphous silicon depositions, such as Chemical Vapor Deposition (CVD) as a thin film.

1.12 Annealing Process Affects the Efficiency

The amorphous silicon has a large number of defects and impurities, especially at the interface of p-i and n-i as per the defect model (Powell & Deane, 1996). This density increases near the surfaces as compared to the bulk; therefore, the probability of recombination increases at the surface. If the device is passed through the annealing process when it is in reverse biasing, then the hydrogen atoms move towards the interface of the device and the defects will be reduced (Carlson et al., 1999; Dutta & Murthy, 1997). These states at the interfaces cause open circuit limitation and modify the interface by buffer layer, increasing the open circuit voltage (Jiang et al., 2000; Wang et al., 2000). By using these techniques, the recombination probability can be decreased, especially near the interface, which may really affect the efficiency of the device.

1.13 Efficiency Verses Cost

The efficiency is the amount of current (e) generated by single photon of light. It measures the output of electrical energy of the device for a given amount of light energy (photon) at input. The typical efficiency of amorphous silicon is about 3 to 6%; mono-crystalline silicon has 12 to 15%; and polycrystalline silicon has 10 to 13% (Nema, Nema, & Rangnekar, 2009). The lower efficiency means that more PVs are needed to compensate for the output; however, by introducing some new techniques, we can improve the efficiency at reduced cost. Though the cost of high grade silicon continues to fall as the fabrication procedures become steadily improved, the huge demand in the electronics integrated application makes it worthy and valuable at the same time.
1.14 Why Simulation Is Important

Simulation is an important tool in technology that enables us to assess, design, and model a system or device before significant time and cost has been invested. It provides insights into the designing of a device and its behavior so the model can be improved without physical measurements. Simulations are being increasingly emphasized in microelectronics and device fabrication. Different design and simulation software tools are being used in the fabrication of semiconductors to investigate the parameters of devices such as the diffusion of dopant atoms, oxidation, ion implantation, and etching and deposition of thin films. These tools can easily calculate the transport of carriers and associated field distribution due to the applied external field by using any suitable software. AFORS-HET for 1-D and Lumerical FDTD/DEVICE have been used for the simulation in this study. Both provide a wide range of affordable technologies and a better platform for simulation and control. The Lumerical FDTD/DEVICE is mostly used for studying, designing, and modeling of PVs and other electronic devices. The rise of semiconductor electronics has increased the demand for transistors used on an IC. Results to increase data processing and speed that facilitated to store and process more data inexpensively in today’s chip. The synergistic combination of modeling and simulation tools, Technology Computer-Aided Design (TCAD), is also a robust platform with the critical analysis and detailed understanding at various levels, including system and circuit design, device engineering, process development, and integration into manufacturing (Liebmann et al., 2001). The Lumerical FDTD/DEVICE is the latest tool that is specifically used for simulation and design of solar cells. It can simulate the electrical characteristic of heterojunction semiconductor devices. It solves Poisson’s equation coupled with the charge carrier continuity equation. It was originally written to model a wide variety of solar cells for different materials. Within this platform, known parameters of a particular material (e.g., band gap, mobility, and carrier concentration) are used to investigate the unknown parameters with better control and assessment.
CHAPTER 2

Literature Review
literature review

The improvement in the efficiency and in solar energy conversion technologies are going towards saturation, but there is still the need for advancement in this energy portfolio. Researchers are continuously proposing and designing efficient and cost-effective devices, especially focusing on Si technology as the most economical technology at a larger scale. Here we have a brief discussion about the literature and some of the previous research work that is relevant to this research study, the amorphous Si solar cell.

The first concept of an amorphous and microcrystalline tandem solar cell was introduced by a research group in IMT (Institute of Microtechnique, University of Neuchatel). It was n-i-p-n-i-p structured. According to Goetz, Torres, Pernet, Meier, Fischer, Kepper, and Shah (1996), this structure improved the deposition of mid-gap, intrinsic microcrystalline silicon (µc-Si:H), using a gas purifier method. Goetz introduced the concept of a NIP amorphous and microcrystalline silicon single junction solar cell. An aluminum sheet was used as the substrate for silicon thin film deposition. Goetz et al. (1996) had used the flat aluminum substrate with a thin layer of antireflection coating to trap light back into the solar cell. The concept of an antireflection layer with a flat substrate used for amorphous silicon solar cell have its limitation for extended range of spectral response. This study of Goetz achieved the best initial efficiencies for each category of n-i-p cell on a flat substrate: 8.7% for amorphous silicon single junction, 4.9% for the microcrystalline silicon single junction cell, and 9.25% for the micromorph tandem cell.

The potential and efficiencies of a silicon heterojunction solar cell were studied by Descoeudres, Holman, Barraud, Morel, Wolf, and Ballif, (2013) on n- and p-type c-Si wafers. The thin intrinsic a-Si:H layer between the p+ / n+ and c-Si (n- or p-type) provided an improvement in c-Si surface passivation. In the low injection range, the p-type wafer suffers from reduced minority carrier lifetime due to the asymmetric interface defect, which leads to a lower fill factor than the n-type wafer cell. These losses were minimized by high quality passivation layers. The
high open-circuit voltages \( (V_{oc}) \), 735 mV on n-type and 726 mV on p-type, were obtained for both types of wafers. The highest aperture-area certified efficiency obtained on a 4cm\(^2\) cell were: 22.14\% on n-type wafer (with \( V_{oc} = 727 \) mV, \( FF = 78.4\% \)) and 21.38\% on p type wafer (with \( V_{oc} = 722 \) mV, \( FF = 77.1\% \)), respectively. This investigation (Descoeudres et al., 2013) showed that the heterojunction technique can perform on high quality p-type as well as on n-type wafers. According to this study, this is the highest efficiency ever reported for a full silicon heterojunction solar cell on a p-type wafer with highest open circuit voltage and with a favorable fill factor.

The aim of most and the latest research is to produce a high efficiency thin-film tandem solar cell at lower cost. With the same aim, Lee, Kim, Yoon, Song, and Park (2004) investigated the operation properties of a-Si:H, \( \mu \)c-Si:H and a-Si: H/\( \mu \)c-Si:H tandem solar cells with variation in the front TCO, structure of back reflector, and thickness of bottom cell. This investigation shows that the short circuit current density \( (J_{sc}) \) of the cells are highly dependent on light trapping and current matching techniques by varying the above said parameter. The ZnO was used as the front TCO. The ZnO, also at the intermediate layer, was used to reduce the junction effect between the cells and support the tunneling of the carrier. The thicker i-layer at the bottom of the cell was deposited to obtain high current density; however, it reduced the \( V_{oc} \) and \( FF \) due to the result of degradation of thin film quality by increasing the deposition rate. This study has achieved a maximum 9.8\% efficiency with ZnO:Al texture, back contact of ZnOIAg, and with bottom i-layer thickness of 1.8\( \mu \)m.

Amorphous and polycrystalline semiconductor thin films have great potential for decreasing the cost of photo cells. In the study of Morales-Acevedo (2006), the investigation is on a totally different type of photovoltaic. It has different characteristics and is fabricated on crystalline silicon for which the carrier-transportation and behavior is usually clearly known. The design of a heterojunction solar cell was made on less known polycrystalline material. Before this study, several physical aspects of the behavior of a polycrystalline thin film
solar cell was studied and finally a suitable design was made. The recombination at the grain boundary and its effect on the short current density as a function of the crystallite size on the active material was assessed. On the basis of this analysis, the appropriate thickness of each layer and its resistivity was measured. Finally, these considerations and theories were applied to CdS/CdTe heterojunction solar cells by further considering the typical properties of active material CdTe thin film. If the average CdTe layer grain size is less than 0.5µm, a CdTe film of thickness of 1µm is enough; on the other hand, if the grain size is the same but the CdTe layers have a high intrinsic resistivity, an n-i-p structure solar cell could be designed. If the grain size is 1µm, then the thickness of the solar cell should be 2-5 µm thick with suitable resistivity to achieve high $V_{oc}$ and high $J_{sc}$.

In this study, Sritharathikhum, Moollakorn, Kittisontirak, Limmanee, and Sripapha (2011) prepared high quality wide band gap hydrogenated intrinsic silicon oxide (i-a-SiO:H) film by 60MHz VHF-PECVD. The effect of plasma power density on the defect density of the film was investigated. The defect density defines the quality of silicon thin film and it was found that defect density increases with the increase of plasma power density. The i-a-SiO:H was fabricated to study the effect of plasma power density on i-a-SiO:H deposition and its performance. The study results showed that the conversion efficiency was improved from 6.8% to 7.3% due to the increase in full factor by reducing plasma power density from 50.0 to 30.3 mW/cm$^3$. Also, as compared to the conventional i-a-SiO:H solar cell, the peak spectral response was shifted to the short wavelength region (400-600nm) from (550-600nm). According to these results, it was recommended that the i-a-SiO:H film be applied on top of multi-junction solar cell in order to improve the light absorption in the short wavelength region.

The amorphous (a-Si: H) and microcrystalline (µc-Si:H) silicon thin film had been used in solar cells as the main absorber material and for light trapping. It also plays an important role in its performance. Müller, Rech, Springer, and Vanecek (2004) investigated efficient light trapping techniques by using textured transparent conductive oxide (TCOs) as light scattering, highly conductive, and
transparent front contact in a silicon p-i-n structure. The ZnO:Al film was prepared by magnetron sputtering and subsequently textured by a wet-chemical etching step. The influence of electrical, optical, and light scattering properties of ZnO:OAl front contact and the role of the back reflector were studied in experimentally prepared a-Si:H and μc-Si:H solar cells. This model was applied to develop a roadmap for further stable efficiency up to 15% as in an amorphous or microcrystalline tandem cell. The incorporation of an efficient layer of an intermediate reflector between the a-Si:H top and μc-Si:H bottom cell was important. The front TCO has low absorption of light while from the back, the light is ideally scattering back with low losses. Finally, the ZnO front contact had been upgraded by a low cost mid-frequency reactive sputtering technique to prepare an industrial size substrate area. Both an experiment and theoretical simulation had been used to model the design and showed absorption losses and light scattering properties of the front TCO that influence the device efficiency. A ZnO/Ag double layer was used as a highly reflective back contact in this design.

TCO always has an important role in optical absorption in the case of thin film solar cell. The thin film does not have sufficient thickness to absorb the light, with energy greater than the band gap, in one pass. Therefore, TCO facilitates the nearly complete absorption of light. Different techniques have been applied by varying band gap or using multiple junction solar cells; however, the deterioration of electronic quality of new materials has many limitations. Rath, Liu, De Jong, De Wild, Schuttauf, Brinza, and Schropp (2010) investigated texture etched ZnO:Al as compared to other transparent conductive oxides such as Asahi glass SnO2:FTCO in case of a nano-crystalline silicon solar cell. The ZnO:Al layer was made at room temperature by changing the stress from tensile to compression with the increase in substrate temperature of sputter deposition and rms roughness. The haze of the film was seen to have a correlation with the stress of the film. The technique provided the best combination of electrical properties and scattering properties of the textured etched layer. A current density of 24 mA/cm³ was achieved with this technique for an nc-Si cell. For the texturing to make a rough ZnO:Al TCO layer
for a solar cell on plastic, an additional step of embossing the plastic before the sputter deposition of the ZnO:Al layer was employed to reduce undue stress. For the back reflector, use of thick and low doped (0.5% Al) ZnO in combination with a white reflector, instead of metal, is a good solution for plasma absorption loss. In the case of substrate type solar cells on plastics, the ZnO:Al layer that is used as a back reflector as well as a barrier layer, was made to be thin and under a low stress condition. The device, n-i-p a-Si solar cell, finally has overall efficacy of 6%.

Simulation and the latest technology has also contributed to the improvement of solar cell technology. Haque, Quuddus, Ferdaous, and Hoque (2013) studied the efficiency variation with the change of device parameter using Adept 1D simulation and an $Al_{0.7}Ga_{0.3}As/Al_{0.48}In_{0.52}As$ hetero-junction solar cell. The device used an n-typed top layer $Al_{0.7}Ga_{0.3}As$ as the emitter, a p-type middle layer $Al_{0.48}In_{0.52}As$ as the base, and a p-type bottom layer $Ga_{0.67}In_{0.33}As$, which was highly doped and acted as a passivation layer. Ge was used as the structure (p-doped). Variation in efficiency was plotted by changing the thickness of layers and carrier concentration. The variation curve, from two optimum designs, produced efficiencies of 19.57% and 20.56%, respectively.

Serin (1998) studied the reverse bias annealing effect on the density of states in a hydrogenated amorphous silicon (a-Si:H) pin diode. To find the effect of reverse bias thermal annealing on the density of states around the mid-gap of the intrinsic region in p-i-n structure a-Si:H, first the junction capacitance was measured at an annealing temperature of 23 to 155 °C. Then, the density of states around the mid-gap intrinsic region was determined by three different capacitance techniques. The mid-gap density of states of intrinsic layer first decreased with increasing annealing temperature up to 130 °C, then increased again. The results of this study were interpreted with the defect pool model.

Depauw, Qiu, Van Nieuwenhuysen, Gordon, and Poortmans (2011) studied high quality silicon film without resorting to costly epitaxy. The difficulty in this technique is producing etching-controlled and regular pores in silicon in a cost effective way and in developing a process that is capable of handling a micro-
thin material. The process involves lifting off of a high quality monocrystalline by annealing of cylindrical macropore arrays in silicon. The energy conversion efficiency of 1 μm-thin Epifree cells was improved from 2.6 to 4.1% with the help of a-Si layer as the rear-side passivation. The thinness of the film leads to a decrease in rear-side reflectivity by a-Si and aluminum. These issues indicate that an alternative surface passivation should be developed. As a result of this concept, the material was thickened by modifying the macropore array dimension, up to 2 to 4 μm thick material over a 1cm² area. The efficiency of such a cell is expected to increase by adding this thicker material.

Gaubas, Čeponis, Kalendra, Kusakovskij, and Uleckas (2012) assessed the technique of Barrier Evaluation by Linearly Increasing Voltage (BELIV) and applied this technique to a Si solar cell and irradiated PIN diode. They presented the BELIV technique as a tool for fast evaluation of barrier parameters in the junction structures. The technique has been recommended to examine the structure of irradiated particle detectors, PIN diodes, and solar cells. The components of barrier capacitance charging and generation/recombination were analyzed. Different situations of the impact of deep center defect on barrier and diffusion capacitance changes were studied. It was shown that the built-in full depletion (insulating state) is inherent for an Si diode doped with 10¹² cm⁻³ donor density and irradiated with hadron fluences above 10¹⁴ cm⁻². This technique, which is used for further analysis of barrier quality in solar cells and particular detectors fabricated on silicon material, was demonstrated.

The performance of thin film solar cells are limited by poor light absorption and carrier collection. Wang, Wu, Reinhardt, Lu, and Chen (2010) realized large broadband and polarization-insensitive light absorption enhancement via integrating with thin metallic nanogratings. They used simulation and proposed three mechanisms (the Febry-Perot resonance, SPPs resonance, and planer waveguide coupling) that were responsible for such a huge improvement. This study showed up to 30 % broadband absorption enhancement over the solar spectrum as compared to bare thin film cells. This unique solar cell has no proper
shape or geometry; therefore, the cost could be better balanced. Besides the focus on a-Si, it can be extended to other solar active materials such as CdTe and other organic materials.

Most thin film solar cells need a light trapping technique, which is predominately based on depositing the solar cells on rough surfaces. This approach is appreciated and increasingly used; however, current density, open circuit voltage, and fill factor usually decrease with this technique. Söderström, Bugnon, Biron, Pahud, Meillaud, Haug, and Ballif, (2012) proposed the solution for this dilemma and investigated the substrate that decouples the growth interface from the light scattering interface. Moreover, they studied the concept in thin film silicon cells. First, they reviewed the rough versus smooth interface for n-i-p single junction and µc-Si:H cells. Then the benefits of a newly developed substrate decoupled the growth. Scattering and losses at interfaces were investigated in n-i-p triple junction (a-Si:H/µc-Si:H/ µc-Si:H) first time. The conversion efficiencies were initially 13.7% and stabilized at 12.5%.

According to De Wolf, Descoeudres, Holman, and Ballif (2012), the crystalline silicon solar cell achieved a conversion efficiency up to 20% at the industrial level. These solar technologies consist of amorphous and monocrystalline silicon wafers. The main point of these structures is the displacement of highly recombination-active (ohmic) contact from the crystalline surface by insertion of a thin film with a wide band gap. The hydrogenated amorphous silicon film with a few nanometers of thickness has a wider bandgap than c-Si and when in intrinsic form, these films can reduce the c-Si surface state density by hydrogenation. The amorphous silicon films can be relatively easily doped, either n- or p-type, allowing for the fabrication of contacts with record-low values for the saturation current density. The large-area (> 100 cm²) energy conversion efficiencies (up to 23%) were reported by Sanyo Japan for such a device.

Surface passivation is very important for any high frequency solar cell. De Wolf, Andrault, Barraud, Bartlome, Bätzner, Bôle, ... and Holm (2010) focused on the surface passivation mechanism of intrinsic and doped amorphous silicon films.
They assessed the relation between $V_{oc}$ and the surface passivation properties of the thin amorphous silicon layer. The new generation large area PECVD of amorphous silicon was introduced. The new parallel-plate reactor is able to produce silicon films with a uniformity of less than 5%. The silicon surface layer passivation quality was comparable with the best results, with a carrier lifetime of up to 9.6 ms on an n-type polished substrate. The films were adjusted in 2x2 cm$^2$ aperture area solar cells, with a conversion efficiency of 21% on a textured n-type FZ Si substrate.

Biron, Hänni, Boccard, Pahud, Söderström, Duchamp, ..., and Parascandolo (2013) studied tandem amorphous and microcrystalline silicon solar cells with no uniform and asymmetric intermediate reflectors grown in an n-i-p substrate. The different types of substrates with consideration of light trapping properties and their influence on single junction growth were investigated. The most promising back reflector was grown by low pressure PECVD in combination with textured zinc oxide, a silver film for reflection, and a zinc oxide buffer layer. The microcrystalline cell grown on this substrate showed better results with high $V_{oc}$ and fill factor and an efficiency of 10%. After optimization, an n-i-p micromorph solar cell with stabilized efficiency of 11.6% was achieved using 270 nm and 1.7 µm of silicon for the absorber layer of the amorphous top cell and microcrystalline bottom cell respectively.

Nawaz (2011) designed a two-dimensional computer analysis of thin-film amorphous silicon heterojunction solar cells by using commercial TCAD software. He presented the analysis for the thin film based hydrogenated amorphous silicon (a-Si:H) by comparing various absorbing layers, such as a-Si, a-SiGe, a-SiC, and all in combination with a a-Si+ a-SiGe, a-Si/a-SiGe layer and in tandem form. Moreover, he implemented a special surface recombination model, thermionic field emission for transport at heterojunction, and interface trap model at the top and bottom junctions of the heterojunction interfaces. He achieved 10.1% efficiency for a single absorber graded design with 800nm thick multiband absorption. The efficiency of his tandem design is 10.4% with a total absorber thickness of 800nm.
at 1.75 eV and at 1.0 eV for the top a-Si and bottom a-SiGe component cells. His tandem design efficiency has improved, but he has a limitation with his graded design (i.e., absorbing layer of a-Si and a-SiGe graded layers).

Moustafa and Boumediene (2013) investigated the doping concentration and thickness of different layers in the heterojunction with an intrinsic thin layer solar cell (HIT). They used AFORS-HET (Automate for Simulation of Heterostructures) to assess the ZnO/a-Si:H(n) / a-Si:H(i) / c-Si:H(p) / a-Si:H(p)/Ag. They showed that a recorded efficiency of 28.1% could be obtained with relevant parameters Voc = 774.22nV, Joc = 42.40 mA/cm², and FF = 85.57%. The results are obtained for 5nm, 3nm, and 150nm, of a-Si:H(n) emitter layer, a-Si:H(i) buffer layer, c-Si(p) absorber layer, and the a-Si:H(p) back surface field layer. The doping concentrations 3 x 10¹⁹ cm⁻³, 8 x 10¹⁶ cm⁻³, and 8 x10¹⁹ cm⁻³ were maintained.

Hernandez-Como and Morales-Acevedo (2010) simulated the HIT solar cell by using AMPS-1D and discuss the modification required to upgrade this software, especially regarding interface and high interface density of states as presented in amorphous silicon and in crystalline silicon hetero-junctions. Moreover, they discuss the approach to develop silicon layers at low temperature 300°C with the purpose of passivating the silicon surface and avoiding the degradation suffered by silicon when processed at high temperature 800°C. Their results show that it is possible to achieve larger efficiencies than 22-23% if c-Si surface passivation is improved by depositing a high quality amorphous Si layer so the total density of states will be reduced to 5 x 10¹⁰ cm⁻². Even with total density of states at interface 1 x 10¹¹ cm⁻², a solar cell can be used for good results.

Lisheng, Fengxiang, and Yu (2011) analyzed the heterojunction with a thin intrinsic layer solar cell. The efficiency of TCO/a-Si:H (n) / a-Si:H (i) / c-Si(p) /uc-Si(p⁺)/ Al was analyzed with AFORS-HET (Automate for Simulation of Heterostructures) software. It was found in this paper that increasing the n layer thickness causes the short spectrum response and the short-circuit density of solar cell to decrease; the insertion of an intrinsic a-Si(i) layer reduces the defect density of states at the interface of the solar cell. If the interface has a lower density of states,
then the thickness should be no more than 5 nm. The back-surface field has little effect on the conversion efficiency of the solar cell. The final parameters of the HIT solar cell is $V_{oc} = 678.9 \text{mV}$, $J_{sc} = 37.35 \text{mA/cm}^2$, $FF = 83.97\%$, and Efficiency = 21.29\%.

Nawaz and Ahmed (2012) assessed the influence of absorber doping for a a-Si:H/a-SiC:H/a-SiGe:H -based thin film solar cell using a Two-dimensional Computer Aided Design (TCAD) tool. Various parameters of the absorber layer have been studied, i.e., doping and thickness, and realistic predictions were made regarding the device simulation. The necessary models – surface recombination, thermionic field emission tunneling model for carrier transport at heterojunction, Schokley-Read Hall recombination model, auger recombination model, band gap narrowing effects, doping and temperature dependent mobility model, and Fermi-Dirac statistics – were implemented. A single absorption layer with graded design has an efficiency of 10.1% for 800 nm thick multiband absorption. The tandem design has the efficiency of 10.4% with a total 800nm thickness. The moderate n doping in the absorbing layer helps to improve efficiency and p doping in the absorber degrade efficiency due to the decrease in the Voc and fill factor of the device.
CHAPTER 3

Theoretical and Computational Models of

Lumerical DEVICE/ FDTD and AFORS-HET
Theoretical and Computational Models of AFORS-HET and Lumerical

The AFORS-HET (Automat For Simulation of Hetero Structures) is used for numerical simulation of an a-Si heterojunction solar cell, whereas the Lumerical DEVICE/ FDTD is a multipurpose designing tool for simulating and optimizing the performance of photonic integrated circuits. The solar cell simulation is divided into two parts. First, the optical simulation: the generation rate \( G(x, t) \) within the solar cell is calculated. This means calculating the total number of excess electrons and holes that are created in unit volume in each second at a particular position \( x \) due to light absorption. It all depends on the model that is chosen to calculate and simulate the effect of internal and external reflection and coherent superposition of light propagation or scattering internally. Second, by electrical simulation: concern for the local total densities of electrons \( n(x, t) \) and holes \( p(x, t) \) and the local potential \( \phi(x, t) \) are calculated within the solar cell. The solar cell is always operated under specific conditions, for example, in an open circuit with some specific external cell voltages or in short circuit conditions. For each condition, internal quantities, band diagram, local recombination rates, local cell current, and local phase shift can be calculated. For electrical simulation, first, the local generation rate \( G(x, t) \) has to be defined so the optical simulation can be calculated later on. Second, the local recombination rate \( R(x, t) \) has to be clearly defined in terms of local unknown variables \( n, p, \phi \), so \( R(x, t) = f(n, p, \phi) \). The recombination models: direct recombination (radiative recombination), indirect recombination (auger recombination), or recombination through the defects (Shockley-read- Hall recombination, dangling-band recombination) can be considered.

To simulate the real values of the measurements, the optical and electrical simulations are continuously measured with certain levels of accuracy by considering different boundary conditions of the predefined problem. The simulation of IV characteristics is calculated by calculating its internal total charge density (the electron and hole current) with respect to the change in external applied voltage.
The technique of heterojunction is used to minimize the contact recombination, by different semiconductors with different band gaps, which are used to form solar absorbing layers for collection of photons. The generated excess carriers in the extracting area are separated by attracting towards the contact. These selective contacts are designed by doping at the edges of the solar cell; as a result, it creates an internal electric field by which the excess carriers are separated and collected at different contacts. The type of contact depends upon the band gap and work function of the semiconductors. A homojunction has no band gap offsets while a heterojunction has the band gap offsets that help to repel the excess charge carriers at contact and have a high open circuit voltage. The diagrams of different contacts are given in Figure 3.1.

![Ideal, Homo, and Hetero Contacts](image)

**Figure 3.1** Schematic sketches of p-type semiconductor absorbing layers which are used to form different types of semiconductor junctions (Stangl, Leendertz, & Haschke, 2010).

For any computer simulating software, it is important to consider the contact recombination and how to handle different types of junction form between the semiconductors. The interface defects and the corresponding interface
recombination $R^{it}(t)$ should be modeled depending on physical assumptions of how to describe the carrier transport.

Device simulation has played a very important role in the technology development process. Some of the important benefits of simulations that can be achieved before designing the physical device are given below:

- Without investing in fabrication, the electrical, thermal, and optical characteristics of semiconductor devices could possibly be studied in depth and well analyzed.
- Static and transient terminal current and voltage can be determined with variations of variables under different conditions.
- The operation of devices can be well understood by predicting the response and behavior of the device by using known parameters such as potential, current density, electrical field, recombination, and generation rate distributions.
- Device design can be optimized for the best performance with the most suitable structural parameters without investing a large amount of money.
- Degradation with time and failure mechanisms, such as decrease in efficiency of a-Si:H solar cell with temperature and with time can be studied.
- Data can be generated to model the generation and to analyze the designing phase before any further processing is established (Hidalgo & Lanchares, 1997, September).

### 3.1 Introduction to AFORS-HET

The AFORS-HET 2.4.1 solves one-dimensional semiconductor equations, Poisson’s equation, and transport and continuity equations for both electrons and
holes with the help of finite differences and under certain conditions, i.e., (1) equilibrium mode, (2) steady state mode, (3) steady state mode with small additional sinusoidal perturbations, (4) simple transient mode, which is used for switching external quantities instantaneously on and off, and (5) general transient mode, which allows for arbitrary change in external quantities.

Multiple physical models can be implemented, but in general, the generation of charge carriers (called the optical model in AFORS-HET) can be defined either by Lambert-Beer absorption, considering rough surfaces and using measured reflection and transmission files, or by considering plain surfaces with incoherent/coherent multiple internal reflections by using the complex indices of reflections for individual layers. The different recombination models can be considered in AFORS-HET, such as radiative recombination, Auger recombination, Shockley-Read-Hall, or dangling-bond recombination, with any defined defect states within the band gap. Super- and sub-band gap generation and recombination can be handled. The following interface models can be defined within this software for heterojunction.

The interface carrier transport can be modeled by either the drift diffusion model or by the thermionic emission model. The tunneling effect via band to trap across the interface can be considered. The following boundary model can be chosen. The metallic contacts can be modeled as flat-band or Schottky life metal/semiconductor contacts, or as metal/insulator/semiconductor contacts. Moreover, insulating boundary contact can also be selected.

All the internal cell quantities, such as band diagram, carrier densities, cell current, phase shift, quasi Fermi energies, and local generation or recombination rate can be calculated by this tool. There are some solar characterization methods, for example, current voltage, transient or quasi-steady-state photo conductance, quantum efficiency, spectral resolved steady-state or transient photo and electro-luminescence, transient or quasi-steady state surface photovoltage, capacitive voltage, impedance/admittance, capacitive temperature, and capacitive-frequency. The front outlook of the software is shown in Figure 3.2.
Figure 3.2 AFORS-HET front outlook (a) without and (b) with further input options.
This program has other options, such as arbitrary parameter variations and multidimensional parameter fitting in order to maximize and match simulated measurements to real experimental data. This is an open source on-demand program and is available online at http://www.helmholtz-berlin.de.

3.2 Basic Input Parameters of AFORS-HET and Associated Physical Models

Both optical and electrical parameters for AFORS-HET are discussed in the following sections.

3.2.1 Optical Parameters.

The incident photon flux is defined as $\Phi_0(\lambda, t)$ which is the total number of photons with certain wavelength $\lambda$, are incident at the time $t$. The total optical generation rate $G(x, t)$ within the semiconductor stack is calculated by calculating the number of total electrons and holes that are created per second, per unit volume, at the time $t$, at the position $x$ due to bend gap absorption. There are two types of optical models available: (1) Lambert-Beer absorption and (2) coherent/incoherent internal multiple reflections. For both models, the dielectric properties of the semiconductor have to be specified with the thickness. For example, the values of complex refractive indices, $\bar{n}_i(\lambda) = n_i(\lambda) - i k_i(\lambda)$ with refractive index $n(\lambda)$ and extinction coefficient $k(\lambda)$ must be provided. If the Lambert-Beer absorption is chosen, a measured reflectivity $R(\lambda)$ of semiconductor stack should be specified. The resulting absorption $A(\lambda, x, t)$ within the semiconductor stack will be calculated with the assumption of Lambert-Beer absorption by using the specified values for $k_i(\lambda)$ and performing the ray tracing in order to account for the texture of the surface with multiple bounces of light within the semiconductor. If the second model, the coherent/incoherent internal multiple reflection, is chosen, then the reflection $R(\lambda)$, transmission $T(\lambda)$, and the absorption $A(\lambda, x, t)$ of the semiconductor are calculated from the values $n_i(\lambda)$ and $k_i(\lambda)$, assuming plain surface within the stack, taking internal coherent multiple reflections into account,
if desired. Both of the models $G(x, t)$ and $A(\lambda, x, t)$ are calculated by integrating the overall wavelength of the incident spectrum. In order to model the optical sub-band gap generation, optical electron and hole capture cross section $\sigma_{n, opt} \neq 0$, $\sigma_{p, opt} \neq 0$ for the Shockley-Read-Hall defect have to be specified.

### 3.2.2 Parameters Related to the Layer and Device

For each semiconductor, all the relevant parameters have to be specified, such as the effective conduction and valance band density of states $N_v$ and $N_c$, thickness of the layer $L$, the electron and hole thermal velocities $v_n$ and $v_p$, the electron and hole motilities $\mu_n$ and $\mu_p$, electron affinity $\chi$, the relative deflective constant $\varepsilon$, doping concentrations $N_d(x)$ and $N_d(x)$, and band gap of the semiconductor. To consider the recombination within the semiconductor, four different recombination models can be chosen: (1) radiative recombination, (2) Auger recombination, (3) Shockley-Read-Hall recombination, and (4) dangling bond recombination. In radiative recombination, the radiative band-to-band rate constant has to be defined $r^{bb}$ (Sze & Ng, 2006). In Auger recombination, the electron and hole auger rate constant $r_{n Aug}$, $r_{p Aug}$ have to be specified (Sze & Ng, 2006). For the Shockley-Read-Hall recombination, the defect density distribution within the band gap of the semiconductor $N_{trap}(E)$ and two capture cross sections $\sigma_n$, $\sigma_p$ and, if needed, two optical capture cross sections $\sigma_{n, opt}$, $\sigma_{p, opt}$ for both carriers have to be specified (Sze & Ng, 2006). For the dangling band recombination, the defect distribution within the band gap of semiconductor $N_{trap}(E)$ with four capture cross sections $\sigma_n^+, \sigma_n^0, \sigma_p^0, \sigma_p^-$ and correlation energy $U$ have to be specified (Sah & Shockley, 1958).

### 3.2.3 Interface Parameters

Interface parameters could be specified by describing three different models for transport of charge carriers: (1) no interface, (2) the drift diffusion model, and (3) the thermionic emission model. To define any interface, an interface defect distribution has to be specified $N_{dtrap}(E)$; otherwise no interface will be considered.
For the drift diffusion model, the carrier transport capture cross sections $\sigma_{n}^{it}$, $\sigma_{p}^{it}$ and the thickness of the interface have to specified. The basic concept of drift diffusing is the same as the one applied for the bulk layer of the semiconductor. For the thermionic emission interface model, four capture cross sections $\sigma_{n,1}^{it}$, $\sigma_{n,II}^{it}$, $\sigma_{p,1}^{it}$, $\sigma_{p,II}^{it}$ and a very thin interface have to be specified. Sometimes, four additional optical capture cross sections $\sigma_{n,1}^{it, opt}$, $\sigma_{n,II}^{it, opt}$, $\sigma_{p,1}^{it, opt}$, $\sigma_{p,II}^{it, opt}$ have to be defined. Finally, the transport across the interface is treated according to the thermionic theory (Sze & Ng, 2006).

### 3.2.4 Boundary Parameters

At the boundary of the semiconductor stack, normally a metal, or in some specific conditions, insulator contacts are designed. Four different models are defined to design the boundary interfaces: (1) flat band (which is a metal and semiconductor contact), (2) Schottky metal/semiconductor contact, (3) insulator contact, and (4) metal/insulator/semiconductor contact. For the flat band model, no band bending will be induced. The carrier surface recombination velocities have to specify $s_{n, front/back}$, $s_{p, front/back}$. The additional work function $\phi_{front/back}$ of the metal contact has to be given in the case of the Schottky metal/semiconductor contact. The depletion or the accumulation regions will be formed according to Schottky theory (Sze & Ng, 2006). The interface defect distribution $N_{\text{trap}} (E)$ is required to be specified for the metal/insulator/semiconductor contact model with the capture cross sections $\sigma_{n}^{it}$, $\sigma_{p}^{it}$ (Kronik & Shapira, 1999).

### 3.2.5 Circuit and External Parameters

For any model circuit elements, such as series resistance $R_s$, shunt resistance $R_p$, parallel capacitance $C_p$, and in metal/insulator/semiconductor contact, a series of capacitance $C_s$ can be specified. The elements need to be specified if internal voltage $V_{int}$ and the current $I_{int}$ of stacks are different from external applied values.

The external parameters, which are externally applied to the device under certain considerations, are defined and can be easily varied. These external
parameters are temperature $T$ of the device, a spectral photon flux $\Phi_0(\lambda, t)$, externally applied cell voltage $V_{\text{ext}}$, and external cell current $I_{\text{ext}}$.

### 3.3 Mathematical Description and System of Equations Solved for AFORM-HET

The differential equations and corresponding boundary values are stated in the following paragraphs. Any arbitrary stack of semiconductor can be modeled with the Poisson equation and the transport and continuity equations. These equations can be solved for calculating charge carriers. At the boundaries and at interfaces, these physical models can be defined differently. These are a highly non-linear coupled system of equations with respect to time and space derivatives. The electron density $n(x, t)$, hole density $p(x, t)$, and electrical potential $\phi(x, t)$ are independent variables, for which this system of differential equations is solved. The numerical outline is used from Selberherr (2012) to linearize the problem with Kundert, and Sangiovanni-Vincentelli (1988).

It can be solved for different calculation modes: (1) Internal quantum efficiency (IQE) calculation mode, which describes the thermodynamic equilibrium at a given temperature; (2) DC calculation mode, which describes the steady state conditions under an external applied voltages or current, and/or illumination. In both of these models, all time derivatives are vanished, resulting in a simplified system of differential equations. The system of differential equations is solved for time independent, but position dependent functions, $n^{E\text{Q}DC}(x)$, $p^{E\text{Q}DC}(x)$, and $\phi^{E\text{Q}DC}(x)$.

\[
\begin{align*}
n(x, t) &= n^{E\text{Q}}(x), & n(x, t) &= n^{DC}(x) \\
p(x, t) &= p^{E\text{Q}}(x), & p(x, t) &= p^{DC}(x) \\
\phi(x, t) &= \phi^{E\text{Q}}(x), & \phi(x, t) &= \phi^{DC}(x)
\end{align*}
\]

(3) The AC calculation mode, which describes small additional sinusoidal modulation of the external applied voltage/illumination. Dependencies can be
described by the sinusoidal modulations and all time dependent quantities are then modeled with complex numbers (marked as ~), which allows determining the amplitude and phasing shift between them. The system of independent differential equations can be defined as

\[ n(x, t) = n^{DC}(x) + \tilde{n}^{AC}(x) e^{i\omega t} \]
\[ p(x, t) = p^{DC}(x) + \tilde{p}^{AC}(x) e^{i\omega t} \]
\[ \phi (x, t) = \phi^{DC}(x) + \tilde{\phi}^{AC}(x) e^{i\omega t} \]

(4) The TR (transient) calculation mode, which describes the transient changes of the system due to general time dependent changes of external applied quantities. The system starts in steady state with DC mode simulation; then any arbitrary evolution in time of the external applied voltage or current and/or illumination can be specified by providing appropriate files. The functions \( n(x, t) \), \( p(x, t) \), and \( \phi(x, t) \) during and after externally applied voltage are calculated.

3.3.1 Optical Calculation: Super Band Gap Generation Models

The generation rate \( G_n(x, t) \), \( G_p(x, t) \) of electrons and holes due to photon absorption are divided into two types, the super-band gap generation (\( E_{\text{photon}} = \frac{hc}{\lambda} \geq E_g \)) and sub-band gap generation (\( E_{\text{photon}} = \frac{hc}{\lambda} \leq E_g \)). In this model, only the super-band gap generation rate is calculated as it is independent of local particle densities \( n(x, t) \), and \( p(x, t) \). The sub-band gap generation depends on the local particle densities and must therefore be calculated within the electrical modeling part. The optical super-band gap generation is equal for electrons and holes and is considered as \( G(x, t) = G_n(x, t) = G_p(x, t) \). Two optical models are available to be adapted: Lambert-Beer absorption and coherent/incoherent internal multiple reflections. The Lambert-Beer model treats surface texture and multiple internal boundary reflections but neglects the coherent effect. It is best suited for a water-based crystalline silicon solar cell. The second model is applied for a plain surface.
Lambert-Beer Absorption

It allows multiple tracing for backward travelling of the incoming light but disregards coherent interference. Measured reflectance and the absorption file of illuminated contact $R(\lambda)$ and $A(\lambda)$ can be loaded or constant values can be used. The incoming spectral photon flux $\Phi_0(\lambda, t)$ is measured with respect to the contact absorption and reflectance; for example, the photon flux incoming through the first semiconductor layer is given by $\Phi_0(\lambda, t) R(\lambda) A(\lambda)$. For tracing the light extended path caused by a textured surface, the incident angle $\delta$ of incoming light can be adjusted. For silicon, the textured wafer with $<111>$ direction, the angle is $\delta = 54.74^\circ$, and for a normal plane $\delta = 0^\circ$. The angle $\gamma$ by which the light travels through the layer stack depends on the wavelength of the incoming light and is calculated by Snell’s law.

$$\gamma(\lambda) = \delta - \left\{ \sin(\delta) \frac{1}{n(\lambda)} \right\}$$

The $n(\lambda)$ depends on the refractive index of the first semiconductor layer at the illuminated side. Photon absorption is then calculated from the spectral absorption coefficient $\alpha_\lambda(\lambda) = 4\pi k(\lambda)/\lambda$ of the semiconductor layer corresponding to the position $x$ within the stack, which is calculated from the provided extinction coefficient $k(\lambda)$ of the layer. The electron/hole generation rate for the super-band gap in a one single run through the layer stack (no multiple passes) is given by

$$G(x, t) = \int_{\lambda_{\text{min}}}^{\lambda_{\text{max}}} d\lambda \ \Phi_0(\lambda, t) R(\lambda) A(\lambda) \alpha_x(\lambda) e^{-\frac{\alpha_\lambda(\lambda) x}{\cos(\gamma)}}.$$  

The $\lambda_{\text{max}}$ and $\lambda_{\text{min}}$ values are generally provided by the loaded spectral range of incoming spectral photon flux $\Phi_0(\lambda, t)$. However, the $\lambda_{\text{max}}$ is updated to ensure that only the super-band gap generation is considered $\lambda_{\text{max}} \leq \frac{hc}{E_g}$.

Optical Model: Coherent /Incoherent Internal Multiple Reflections

The absorption within the semiconductor stack after multiple reflections can be calculated by this model. Additionally, non-conducting optical layers in front of
the front contact and behind the back contact of the solar cell can be assumed to be an effect, such as the effect of antireflection coatings.

The reflectance, transmittance, and absorption of all layers (optical layers and the semiconductor layer) are calculated by using the concept of complex Fresnel amplitudes. Each layer can be specified to be optically coherent or optically incoherent for a particular light beam (incident light). For the coherent effect, the incoming illumination $\Phi_0(\lambda, t)$ is modeled by an incoming electromagnetic wave, with the complex field component $\hat{E}_0^+(\lambda, t)$. This wave travels from the front side in a positive direction towards the back contact, having $\Phi_0(\lambda, t) = \text{Const} |\hat{E}_0^+(\lambda, t)|^2$ or in the opposite direction, tracing as $\hat{E}_0^-(\lambda, t)$ from back contact towards front contact. The complex electric field components of the travelling wave are retraced according to the Fresnel formulas, and thus the resulting electromagnetic wave $\hat{E}_0^+(\lambda, t)$ at any position $x$ within the layer is calculated. An incoherent layer is modeled by coherent layer calculations of several electromagnetic waves within that layer by specifying the integer $N$ (incoherence interactions no) by assuming some phase shift and averaging over the resulting electric field components.

3.3.2 Electrical Calculation – Bulk Layers: Semiconductor Bulk Models

Poisson’s equation and transport equations for electrons and for holes are to be solved in one dimension for the bulk of each semiconductor layer. There are two models available in this mode: (1) standard semiconductor and (2) crystalline silicon. For the first model, all bulk parameters, as specified in Section 3.2.2 (layer parameters), have to be defined and adjusted individually. For the second model, the crystalline model, most input parameters for crystalline silicon are calculated from the few remaining input parameters, such as defect densities $N_D(x)$, $N_A(x)$, $N_{\text{trap}}(x)$ of crystalline silicon. Band gap narrowing and doping dependence of the mobility or Auger recombination of crystalline silicon are needed to explicitly model. Within each layer, functional dependence in space can be defined for doping densities $N_D(x)$, $N_A(x)$. The input parameters can be selected as constant,
linear, exponential, Gaussian-like, or error function like, decreasing or increasing as a function of the space coordinates $x$.

**Bulk Model: Standard Semiconductor**

The doping densities $N_D(x), N_A(x)$ at position $x$ of a fixed donor or acceptor state within any cell are supposed to always be completely ionized and defects $N_{\text{trap}}(x)$ at any position with specific energy $E$ within the band gap of the semiconductor can be locally charged or uncharged within the system. These defects can be defined as acceptor-like Shockley-Read-Hall defects, donor-like Shockley-Read-Hall defects, or dangling bond defects, depending on the defect-type chosen, which can be empty, singly occupied with electrons, or even doubly occupied with electrons (in case of the dangling band defect). Acceptor-like Shockley-Read-Hall defects are negatively charged if occupied or neutral if empty. Donor-like Shockley-Read-Hall defects are positively charged if empty, neutral if singly occupied and negatively charge if double occupied.

The Poisson equation, which is to be solved within each layer, is as given

$$\frac{\varepsilon_0 \varepsilon_r}{q} \frac{\partial^2 \phi(x,t)}{\partial x^2} = p(x, t) - n(x, t) + N_D(x) - N_A(x) + \sum_{\text{trap}} \rho_{\text{trap}}(x, t)$$

where $q$ is the electron charge and $\varepsilon_0, \varepsilon_r$ are absolute and relative dielectric constants. $\rho_{\text{trap}}(x, t)$ will depend on the defect type of the defect under consideration and on local particle densities $n(x, t)$, and $p(x, t)$. Further, it is defined by the trap density distribution function $N_{\text{trap}}(E)$ of the defect, specifying the number of traps at energy position $E$ within the band gap and by some corresponding defect occupation function $\int_{0,\text{trap}}^{\text{SRH}} (E, x, t), \int_{1,\text{trap}}^{\text{SRH}} (E, x, t), \int_{0,\text{trap}}^{\text{DB}} (E, x, t), \int_{1,\text{trap}}^{\text{DB}} (E, x, t), \int_{0,\text{trap}}^{-\text{DB}} (E, x, t)$, defining the probability that a trap with an energy $E$ within a band gap is empty or occupied with a single or double electron.

The one-dimensional equations of continuity and transport for electron and holes, which have to be solved within each layer are
\[-\frac{1}{q} \frac{\partial j_n(x,t)}{\partial x} = g_n(x,t) - r_n(x,t) - \frac{\partial}{\partial t} n(x,t)\]

\[+ \frac{1}{q} \frac{\partial j_p(x,t)}{\partial x} = g_p(x,t) - r_p(x,t) - \frac{\partial}{\partial t} p(x,t)\]

Both super-band gap generation rates \(G_n(x,t), G_p(x,t)\), are determined by optical modeling and the recombination rates \(R_n(x,t), R_p(x,t)\) are described in the next section. The electron and hole currents \(J_n(x,t), J_p(x,t)\) are derived by the gradient of the corresponding quasi-Fermi energy \(E_{Fn}(x,t), E_{Fp}(x,t)\). The position-dependent Fermi energies and the corresponding local electron and hole currents are defined with the help of the Maxwell-Boltzmann approximation for the Fermi-Dirac distribution function.

\[E_{Fn}(x,t) = E_C(x) + kT \ln \frac{n(x,t)}{N_C(x)} = -q\chi(x) + q\varphi(x,t) + kT \ln \frac{n(x,t)}{N_C(x)}\]

\[E_{Fp}(x,t) = E_V(x) - kT \ln \frac{p(x,t)}{N_V(x)} = -q\chi(x) + q\varphi(x,t) - E_g(x) + kT \ln \frac{p(x,t)}{N_V(x)}\]

\[J_n(x,t) = q \mu_n n(x,t) \frac{\partial E_{Fn}(x,t)}{\partial x}\]

\[J_p(x,t) = q \mu_p p(x,t) \frac{\partial E_{Fp}(x,t)}{\partial x}\]

where \(\mu_n\) and \(\mu_p\) are the electron and hole motilities, \(\chi\) is the electron affinity, \(E_C\), and \(E_V\) are conduction and valance band energies, \(E_g\) is the band gap, \(N_C\) is the effective conduction and \(N_V\) is valance band density of states of the semiconductor.

**Recombination**

The recombination of electrons and holes can occur from the conduction band to the valance band directly, called band-to-band recombination, \(R_{n,p}^{BB}(x,t)\) or via Auger recombination, \(R_{n,p}^A(x,t)\). It may also recombine through the defect states located in the band gap of the semiconductor via the Shockley-Read-Hall recombination \(R_{n,p}^{SHR}(x,t)\), or via dangling bands \(R_{n,p}^{DB}(x,t)\). The net result of total recombination is given as
\[ R_{n,p}(x, t) = R_{n,p}^{BB}(x, t) + R_{n,p}^{A}(x, t) + R_{n,p}^{SHR}(x, t) + R_{n,p}^{DB}(x, t). \]

**Optical Sub-Band Gap Generation**

Optical sub-band gap generation means \((\hbar c / \lambda < E_g)\) is calculated with the help of Shockley-Read-Hall recombination statistics. A negative electron/hole SHR recombination rate \(R_{n,SHR}(x, t), R_{p,SHR}(x, t)\) means sub-band gap generation of an electron/hole are from the defect state (trap) into the conduction or valance band. These sub-band gap generations are either voltage driven (thermal) or by optical excitation.

The SRH optical emission coefficient \(e_{n, optical}^{trap}(E, x, t), e_{p, optical}^{trap}(E, x, t)\) can be calculated from the optical electron/hole capture cross section \(\sigma_{n, optical}^{trap},\sigma_{p, optical}^{trap}\) as given in the following:

\[
e_{n, optical}^{trap}(E, x, t) = \int_{\lambda_{min}}^{\lambda_{max}} d\lambda \sigma_{n, optical}^{trap} N_C \Phi(\lambda, x, t) \theta(E_c - E - \frac{\hbar c}{\lambda})
\]

\[
e_{p, optical}^{trap}(E, x, t) = \int_{\lambda_{min}}^{\lambda_{max}} d\lambda \sigma_{p, optical}^{trap} N_V \Phi(\lambda, x, t) \theta(E - E_V - \frac{\hbar c}{\lambda})
\]

\(\Phi(\lambda, x, t)\) is the spectral photon flux inside the semiconductor layer; \(\theta(E)\) is the step function; \(\theta(E) = 1\) for all values when \(E \leq 0\) and \(\theta(E) = 0\) for \(E > 0\).

**Radiative Recombination**

The radiative band-to-band rate constant \(r^{BB}\) must be defined in order to balance the radiative band-to-band recombination rates \(R_{n,p}^{BB}(x, t)\); as a result, the electrons and holes are always equal.

\[ R_{n,p}^{BB}(x, t) = r^{BB} \left\{ n(x, t)p(x, t) - N_C N_V e^{-E_g / kT} \right\} \]

When applying the DC or AC calculation mode, the second order term is to be neglected. In the case of the AC calculation mode, it is simplified as
\[ R_{n,p}^{BB} (x, t) = R_{n,p}^{BB} (x, t) + \tilde{R}_{n,p}^{BB} (x) e^{i\omega t} \]

\[ \tilde{R}_{n,p}^{BB} (x) e^{i\omega t} = r_{n}^{BB} n^{DC} (x) p^{\tilde{AC}} (x) + r_{p}^{BB} p^{DC} (x) n^{\tilde{AC}} (x) \]

**Auger Recombination**

The Auger recombination constant is defined as \( r_{n}^{A} \), \( r_{p}^{A} \) and the values of these constants have to be specified in order to calculate the Auger recombination rate \( R_{n,p}^{A} (x, t) \). Again, the resulting electron and holes must be equal.

\[ R_{n,p}^{A} (x, t) = \left[ r_{n}^{A} n(x, t) + r_{p}^{A} p(x, t) \right] \left\{ n(x, t) p(x, t) - N_{c} N_{V} e^{\frac{-E_{g}}{kT}} \right\} \]

When applying the DC or AC calculation mode, the second order term is to be neglected.

**Shockley-Read-Hall Recombination**

The Shockley-Read-Hall recombination requires specifying the characteristics (acceptor-like or donor-like), the capture cross sections \( \sigma_{n}^{trap} \), \( \sigma_{p}^{trap} \), \( \sigma_{n,\text{optical}}^{trap} \), \( \sigma_{p,\text{optical}}^{trap} \), and the energy distribution \( N_{trap} (E) \) of the defect density within the band gap of the semiconductor. Any arbitrary value of defect can be selected with the following energy distributions \( N_{trap} (E) \):

1) Point like distributed in a single energy \( E_{trap} \) within the band gap.
2) Constant distribution within a specific region within the band gap.
3) Exponentially decaying from the conduction or valence band into the band gap.
4) Gaussian distributed within the band gap.

The positive electron hole SRH recombination rate means recombination of an electron and hole from the conduction or valance band into the defect density state (trap); similarly the negative recombination means the recombination due the generation of free charge carriers through the sub-band gap from defect states into conduction or valance band.
Dangling Bond Recombination

In the recombination of dangling band and charged state in amorphous silicon, the most exact description developed by Sah and Shockley (1958) is used. Three occupation functions, \( f_{+,\text{trap}}^D (E, x, t), f_{0,\text{trap}}^D (E, x, t), f_{-,\text{trap}}^D (E, x, t), \) regarding positive, neutral, and negative charged states have to be derived, corresponding to empty, single, or double occupied electronic states. Four capture/emission processes with the capture cross sections \( \sigma_n^+, \sigma_p^0, \sigma_n^0, \sigma_p \) have to be defined. The two transitional energies \( E_0/+, E_+/0 \) are separated by the correlation energy \( U \), which accounts for the fact that the capture-emission process is influenced by the change of the dangling or by rearrangement of the lattice with its surroundings.

Defect Occupation Functions

The probability of any specific defect can be specified by the defect occupation functions \( f_{0,\text{trap}}^{\text{SRH}} (E, x, t), f_{1,\text{trap}}^{\text{SRH}} (E, x, t), f_{+,\text{trap}}^D (E, x, t), f_{0,\text{trap}}^D (E, x, t), f_{-,\text{trap}}^D (E, x, t) \) (either by the Shockley-Read-Hall or dangling band) that traps electrons within the band gap with energy \( E \) in a semiconductor by empty, singly, or doubly occupying. In DC and AC modes, defects can be expressed in terms of local particle densities, \( n_{\text{DC}} (x), p_{\text{DC}} (x), \bar{p}_{\text{AC}} (x), \bar{n}_{\text{AC}} (x) \) while in the TR calculation mode, the defect occupation functions are generally determined by additional differential equations.

a) Shockley-Read-Hall (SRH) Defect Occupation Functions. Shockley-Read-Hall (SRH) defect can be either empty or occupied by an electron, thus

\[
\int f_{0,\text{trap}}^{\text{SRH}} (E, x, t) + \int f_{1,\text{trap}}^{\text{SRH}} (E, x, t) = 1
\]

The \( f_{1,\text{trap}}^{\text{SRH}} (E, x, t) \), SRH defect occupation for electrons will be explicitly stated when using the EQ, DC, AC or the TR calculation mode. The SRH defect occupation function \( f_{0,\text{trap}}^{\text{SRH}} (E, x, t) \) then can be directly calculated. Any local
change in trapped charge stored in the SRH defect must be determined by the
difference between local electron and hole SRH recombination, as given below:

\[
\frac{d}{dt} \rho_{\text{trap}}(x, t) = R_p^{RHB}(x, t) - R_n^{RHB}(x, t)
\]

For the EQ calculation mode, the SHR defect occupation function is defined by the
Fermi-Dirac distribution function that is further
\[ f_{1,\text{trap}}^{\text{SRH,DC}}(E, x) = f_{1,\text{trap}}^{\text{SRH,EQ}}(E, x) \]
which is explicitly determined by the position independent Fermi energy \( E_F \).

\[
f_{1,\text{trap}}^{\text{SRH,EQ}}(E, x) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}}
\]

b) Dangling Band Defect Occupation Functions. The dangling bond
defects can be either empty, single, or double occupied by an electron;
as a result, it is in a positive, neutral, or negative charged state.

\[
f_{+,\text{trap}}^{\text{DB}}(E, x, t) + f_{-,\text{trap}}^{\text{DB}}(E, x, t) + f_{0,\text{trap}}^{\text{DB}}(E, x, t) = 1
\]

For DC and EQ calculations, the occupation functions are given by

\[
f_{+,\text{trap}}^{\text{DB}}(E, x) = \frac{p^0 p^-}{N^+ p^- + p^0 p^- + N^+ N^0}
\]

\[
f_{0,\text{trap}}^{\text{DB}}(E, x) = \frac{p^- N^+}{N^+ p^- + p^0 p^- + N^+ N^0}
\]

\[
f_{-,\text{trap}}^{\text{DB}}(E, x) = \frac{N^0 N^+}{N^+ p^- + p^0 p^- + N^+ N^0}
\]

where,

\[
N^+ = c_n^+ n^{DC} + e_p^+
\]

\[
p^0 = c_p^0 p^{DC} + e_n^0
\]

\[
N^0 = c_n^0 n^{DC} + e_p^0
\]

\[
p^- = c_p^- p^{DC} + e_n^-
\]
where for each defect, $c_n^+, c_p^0, c_n^0, c_p^-$ are the electron/hole capture coefficients for each positive, neutral, or negative charged state, and similarly, $e_n^0, e_p^0, e_n^-, e_p^+$ are the emission coefficients.

3.3.3 Bulk Model-Crystalline Silicon

This model is designed for the use of a semiconductor layer. All input parameters are defined from the doping densities and the defect densities of a crystalline silicon semiconductor. The doping and temperature dependent based material parameters for crystalline silicon are considered here: (1) Temperature dependence of the intrinsic carrier concentration of crystalline silicon; the intrinsic carrier density, (2) Doping dependent mobility of electron and hole, (3) Doping dependence of Auger recombination in crystalline silicon, (4) Doping and SRH recombination in crystalline silicon (SRH life time model), and (5) Doping dependence of the band gap of crystalline silicon (band gap narrowing model). All these models are similar to numerical computer simulation (Clugston, 1997) except for SRH defects, where a certain energy position within the band gap is considered.

3.4 Electrical Calculation – Interface

Each interface between any two semiconductors can be defined by the following three models: (1) No interface model, (2) drift diffusion interface model, and (3) thermionic emission interface.

3.4.1 Interface Model – No Interface

Any default current of charge carriers across the semiconductor interface is assumed by drift diffusion current with no interface defect present at the interface. The drift diffusion model assumes a certain thickness, which is, by default, given in the numerical setting of AFORS-HET. The material properties change within the interface linearly from semiconductor I to semiconductor II. As a result, the net
current of electrons and holes across the heterojunction interface is treated as in the bulk layer of the semiconductor layer.

3.4.2 Drift-Diffusion Interface

The electron and hole current across the interface of the semiconductor is assumed to be driven by drift diffusion, including additional defects present at the interface. The interface states are divided equally at semiconductor I and semiconductor II and can be occupied by electrons or holes from any semiconductor. For the homogeneous distribution of defect density within the interface layer, $N_{it}(E)$ is converted into the homogeneous layer defect density of the interface layer by $N_{it}(E) = \frac{N_{it}(E)}{d_{it}}$ or $N_{i} = (N_{it}(E))^{3/2}$. Thus, half of the defects are recombined in semiconductor I and half are recombined in semiconductor II.

3.4.3 Drift-Thermionic Emission Interface

The model is designed according to Sze and Ng (2006) and Anderson (1988). By using this model, additional defects can be presented at the interface and recombined with electrons and holes from any side of the interface. According to the Anderson theory, the conduction and valance band offsets $\Delta E_C$ and $\Delta E_V$, which determines the energy barrier of the heterojunction interface, to be overcome by the thermionic emission, are given as

$$
\Delta E_C = \chi^{II} - \chi^{I} \\
\Delta E_V = E_g^{II} - E_g^{I} + \chi^{II} - \chi^{I}
$$

The $\Delta E_C$, $\Delta E_V$ is negative if $E_C$ and $E_V$ drops from the left side to the right side of the interface. The thermionic emission currents across the heterojunction interface $J_n^{TE, I \rightarrow II}(t)$, $J_p^{TE, I \rightarrow II}(t)$, $J_n^{TE, II \rightarrow I}(t)$, $J_p^{TE, II \rightarrow I}(t)$ are clearly defined by using the step function, $\vartheta(E)$, $\vartheta(E) = 1$ for all values when $E \leq 0$ and $\vartheta(E) = 0$ for $E > 0$.

$$
J_n^{TE, I \rightarrow II}(t) = v_n^{II} n (\chi^{II}_{it}, t) e^{\frac{|\Delta E_C| \vartheta(-\Delta E_C)}{kT}}, \quad J_n^{TE, II \rightarrow I}(t) = v_n^{II} n (\chi^{II}_{it}, t) e^{\frac{|\Delta E_C| \vartheta(\Delta E)}{kT}}
$$
\[ J_{p}^{TE,I\rightarrow II}(t) = v_{p}^{I} p(x_{it}^I, t) e^{\frac{[\Delta E_V]}{kT} \phi(\Delta E_V)}, \quad J_{p}^{TE,II\rightarrow I}(t) = v_{p}^{II} p(x_{it}^{II}, t) e^{\frac{[\Delta E_V]}{kT} \phi(-\Delta E_V)} \]

So the net electron and hole current across the interface is given as \( J_{n}^{it}, J_{p}^{it} \), where

\[ J_{n}^{it} = J_{n}^{TE,II\rightarrow I}(t) - J_{n}^{TE,I\rightarrow II}(t) \quad \text{and} \quad J_{p}^{it} = J_{p}^{TE,I\rightarrow II}(t) - J_{p}^{TE,II\rightarrow I}(t) \]

In addition to thermionic emission, there are also defect densities that are considered in this model. The recombination of electrons and holes due to defect densities at the interface are calculated with the thermionic emission process.

3.5 Electrical Calculation- Boundaries: Front/Band Contact to Semiconductor Models

In order to collect the current through front and back contact, these contacts are usually assumed to be metallic; however, it may be insulator contact to measure some specific measurements, such as Quasi Steady State Photo-Conductance (QSSPC) or Surface Photo-Voltages (SPV). Four different boundary models for the interfaces between the contact and semiconductor are available in this software: (1) Flat band metal/semiconductor contact, (2) Schottkey metal/semiconductor contact, (3) insulator semiconductor contact, (4) metal/insulator/semiconductor contact. These boundary models serve as boundary conditions for the system of differential equations describing the semiconductor stack.

3.5.1 Boundary Model: Flat-band Metal /Semiconductor Contact

By default, an ideal flat-band metal/semiconductor contact is considered at the boundaries. The interface between the metal front and back contact and the semiconductor is treated as a boundary condition for the different equations describing the semiconductor layers. For each contact, three boundary conditions including potential and electron/hole densities adjacent to the contact have to be stated. Only the effective surface recombination velocities \( S_{n/p, front/back} \) of electrons
and holes need to be specified. The metal work function $\phi_{\text{front/back}}$ of front and back contact is calculated in such a manner that flatband conditions are reached normally. Flatband conditions are calculated within thermal equilibrium EQ calculation mode, DC, AC, and TM calculation modes with external illumination for optical generation of electrons and holes within the band gap.

### 3.5.2 Boundary Model: Schottky Metal/Semiconductor Contact

This model is designed to describe the metal/semiconductor contacts that drive the semiconductor into the depletion or accumulation condition. The metal work function $\phi_{\text{front/back}}$ has to be clearly described in order to fix the majority barrier height of the metal semiconductor contact:

$$\phi_{Bn}^{\text{Schottky}} = q\{\phi_{\text{front/back}} - \chi_{\text{front/back}}\},$$

$$\phi_{Bp}^{\text{Schottky}} = q\{E_g - \phi_{\text{front/back}} - \chi_{\text{front/back}}\},$$

Otherwise, the boundary model will be totally equivalent to the flatband metal/semiconductor boundary model as described above.

### 3.5.3 Boundary Model: Insulator Contact

When the boundary is considered as an insulator, additional interface states need to be defined according to Kronik and Shapira (1999); they are treated the same as the bulk layer but the densities are given in cm$^{-2}$ instead of cm$^{-3}$. For an insulator/semiconductor contact, the three basic boundary conditions are:

$$-\varepsilon_0\varepsilon_r \frac{\partial \phi(x,t)}{\partial x}|_{x_{\text{front}}} - q \sum_{\text{trap}} \rho_{\text{trap}} = 0$$

$$J_n(x_{\text{front}}) - R_{\text{it},n}^{\text{front}} = 0$$

$$J_p(x_{\text{front}}) - R_{\text{it},p}^{\text{front}} = 0$$

### Boundary Model: Metal/Insulator/Semiconductor Contact

By using a metal/insulator/semiconductor (MIS) contact, the insulator capacity $C$ has to be defined. At the insulator/semiconductor interface, additional
interface defects can be defined, which are treated the same as bulk densities given in cm$^2$ instead of cm$^3$, according to Kronik and Shapira (1999). If both boundaries have an MIS contact, then capacities $C_{\text{front}}$, $C_{\text{back}}$ of the front and back boundaries should be defined separately. Moreover, the voltage function $f$ that drops the voltage at the front MIS contact is compared to the fraction that drops at the back MIS contact. The given external voltage is needed to define how the metal layers are charged. The time dependent boundary conditions (AC or TR calculation mode) for the MIS contact are not implemented at the current state.

3.6 Characterization Method Simulated by AFORS-HET

The most common solar cell characterization methods that are simulated with AFORS-HET are current-voltage (IV), quantum efficiency (QE), quasi-steady-state photoconductance (QSSPC), impedance (IMP, ADM, C-V, C-T, C-f), surface photovoltage (ID-SPV, VD-SPV, WD-SPV) and photo-electro-luminescence (PEL).

3.6.1 Measurement Model: Current-Voltage Characterization

This measurement varies the external voltage at the boundaries and plots the resulting external current through the semiconductor stack in order to obtain the current-voltage characteristics of the simulated structure. For each voltage value, the total current though the structure is calculated. This can be done by dark current or under illumination. The measurement model specifies the data point for maximum-power point (mpp), open circuit voltage ($V_{oc}$), and short-circuit current ($I_{sc}$) and calculates the fill factor $FF$ and the efficiency $Eff$ of the solar cell, whereas the illumination power $P_{\text{illumination}}$ in W/cm$^2$ is calculated from the incident photon spectrum.

$$FF = \frac{V_{\text{mpp}}^{\text{mpp}}}{V_{oc}^{\text{oc}}} \quad Eff = \frac{V_{\text{mpp}}^{\text{mpp}}}{P_{\text{illumination}}} = \frac{FF \cdot V_{oc}^{\text{oc}}}{P_{\text{illumination}}}$$
3.6.2 Measurement Model: Quantum Efficiency (QE)

To calculate the quantum efficiency, the semiconductor needs to be illuminated with monochromatic irradiation at a certain wavelength \( \lambda \), and the difference \( \Delta I_{SC}^{irrad} \) of the resulting short circuit current whether or not the additional irradiation is computed. The QE is defined as

\[
QE(\lambda) = \frac{\text{number of electrons in the external circuit}}{\text{number of photons}} = \frac{\Delta I_{SC}^{irrad}}{q \times \text{number of photons}}
\]

Depending on the number of photons, different quantum efficiencies are calculated: (1) external quantum efficiency EQE, (2) internal quantum efficiency IQE, and (3) corrected internal quantum efficiency (IQE1); only photons of the additional irradiation that are absorbed in the semiconductor stack are counted.

3.6.3 Measurement Model: Quasi Steady State Photo-Conductance (QSSPC)

Excess carrier density dependent lifetimes \( \tau_{n_{alt}}(\Delta n) \), \( \tau_{p_{alt}}(\Delta p) \) for the semiconductor stack of the thickness \( L \) under illumination are calculated according to the following equations:

\[
\tau_{n_{alt}}(\Delta n) = \frac{\Delta n}{\Delta G} \quad , \quad \tau_{n_{alt}}(\Delta n) = \frac{\Delta n}{\Delta G}
\]

\[
\Delta n = \left( \int dx \{ n_{\text{illumination}}(x) \} - \int dx \{ n_{\text{dark}}(x) \} \right) / L
\]

\[
\Delta p = \left( \int dx \{ p_{\text{illumination}}(x) \} - \int dx \{ p_{\text{dark}}(x) \} \right) / L
\]

\[
\Delta G = \left( \int dx \{ G_{\text{illumination}}(x) \} - \int dx \{ G_{\text{dark}}(x) \} \right) / L
\]

The average dark and illuminated carrier densities and the average generation rate are calculated by integrating over the whole structure. The total QSSPC measurements of the passivated c-Si wafer are done with the commercially available setup by Sinton Consulting; an effective measure carrier lifetime \( \tau_{qss} \) is calculated as
\[ \tau_{qss} = \frac{\Delta n_{c-Si} \mu_{n_{c-Si}} + \Delta p_{c-Si} \mu_{p_{c-Si}}}{\mu_{n_{c-Si}} + \mu_{p_{c-Si}}} / \Delta G_{c-Si} \]

### 3.6.4 Measurement Model: Impedance, Capacitance (IMP, AMD, C-V, and C-T)

For the metal semiconductor, both boundaries are strictly defined by the voltage controlled. For the time, independent, external DC voltage \( V_{ext}^{DC} \) and AC voltage is superimposed:

\[
V_{ext}(x, t) = V_{ext}^{DC}(x) + V_{ext}^{AC}(x)e^{i\omega t}
\]

where \( V_{ext}^{DC} \) is the amplitude and \( f \) is the frequency, \( \omega = 2\pi f \). The current in the stacks of the semiconductor due to this small amplitude is calculated. The impedance is defined as the complex resistance of the semiconductor stack and the admittance is the complex capacitance of the semiconductor. It can be represented with an equivalent circuit representation by a parallel circuit of conductance \( G \) and capacitance \( C \).

\[
IMP = \frac{V^{AC}_{ext}}{I^{AC}_{ext}}, \quad ADM = \frac{I^{AC}_{ext}}{V^{AC}_{ext}} = G + i2\pi fC
\]

The capacitance can be plotted as a function of external DC voltages (C-V) as well as temperature (C-T).

### 3.6.5 Measurement Model: Surface Voltages (ID-SPV, VD-SPV, WD-SPV)

According to the numerical model used in Sze and Ng (2006) for a steady state surface photovoltaic (SPV) signal, the front contact must be a metal-insulator-semiconductor contact. The semiconductor is illuminated additionally with monochromatic light with certain intensity and certain wavelength. The potential \( \Delta f \) with and without monochromatic illumination at the first grid point and at the back contact at the last grid point is calculated as the net output as an SPV signal:

\[
V_{SPV-front/back}^{SPV} = \Delta \varphi_{front/back} = (\varphi_{front/back}^{illumination} - \varphi_{front/back}^{dark})
\]
The quantities $\varphi_{\text{front}}$ and $\varphi_{\text{back}}$ will vary upon illumination as the potential is fixed either at the front side or at the back side.

### 3.6.6 Measurement Model: Photo Electro Luminescence (PEL)

Upon illumination, externally or when voltages are applied externally, the emitted radiation is calculated according to the general Planks equation (Hidalgo & Lanchares, 1997).

\[
I(\lambda) = 2c \int dx \left\{ \frac{\alpha(\lambda, x)}{\lambda^5} \cdot \frac{1}{\exp\left(\frac{\hbar c}{\lambda} - \frac{E_{\text{Fn}}(x) - E_{\text{Fp}}(x)}{kT}\right)} - 1 \right\}
\]

By taking re-absorption into account, the wavelength dependent emitted intensity to the front and back is calculated by integrating over the whole structure. For any given $\alpha$ and known wavelength $\lambda$, the spectra $I(\lambda)$ of the emitted photon is calculated by the splitting of the quasi-Fermi level of electrons and holes, $E_{\text{Fn}}$ and $E_{\text{Fp}}$. Moreover, the wavelength region for which the emitted intensity is calculated can be selected.

### 3.7 Theoretical Model and Computational Models of Lumerical DEVICE and FDTD

#### 3.7.1 Theoretical Model of Lumerical DEVICE and FDTD

According to the online provided sources (Solutions FDTD, 2016) the FDTD solution calculates absorption per unit area from the divergence of the Potting vector, $P_{abs} = -0.5 \; \text{real} \left( \nabla \cdot \vec{P} \right)$, which is equivalent to $P_{abs} = -0.5 \; \text{real} \left( i \omega \; \vec{E} \cdot \vec{D} \right)$, and finally it is converted into the final desired equation as given $P_{abs} = -0.5 \; \omega \; |E|^2 \; \text{imag} \; (\varepsilon)$. With the help of this equation, where the electric field intensity and the imaginary part of the permittivity are known, the absorption as function of space and frequency can be calculated. The quantities (electric field intensity and the imaginary part of the permittivity) are easily measured in FTDT.
simulation and are used to calculate the light absorption per unit. The number of absorbed photons per unit area is then calculated in FDTD dividing the value \( P_{\text{abs}} \) with the unit energy of photon \( (\hbar \omega) \). \[ g = \frac{P_{\text{abs}}}{\hbar \omega} = -0.5 |E^2| \text{image} (\varepsilon) / \hbar. \]

The total generation rate is calculated by integrating \( g \) over the simulation spectrum. The ideal case, assuming that all absorbed photon generates electron-hole pairs, the photo-generation current can be obtained as, \[ I = e g \] (A/m), where \( e \) is the electron charge. After calculating the total generated current, the short circuit current density \( (J_{\text{sc}}) \) can be calculated by using DEVICE. The quantum efficiency of a solar cell, \( \text{QE} (\lambda) \) is defined as \[ \text{QE} (\lambda) = \frac{P_{\text{abs}} (\lambda)}{P_{\text{in}} (\lambda)}, \] where \( P_{\text{in}} (\lambda) \) and \( P_{\text{abs}} (\lambda) \) are the power of the incident light and absorbed light within the Si solar cell, respectively, at a wavelength \( (\lambda) \). Using the quantum efficiency, integrated quantum efficiency, \( \text{IQE} \), is defined as \[ \text{IQE} = \int \left( \frac{\lambda}{\hbar c} \text{QE} (\lambda) I_{\text{AM1.5}} (\lambda) \right) d\lambda / \int \left( \frac{\lambda}{\hbar c} I_{\text{AM1.5}} (\lambda) \right) d\lambda, \] where \( h \) is Plank’s constant, \( c \) is the speed of light in the free space, and \( I_{\text{AM1.5}} \) the solar spectrum.

**Figure 3.3** Theoretical model of FDTD and Device software
The spectrum details are used from the online source of the Renewable Resource Data Center (RRDC). The efficiency of the device with metal particles is improved compared to without metal contact. The absorption enhancement $G$ and $g(\lambda)$ are defined as $G = \text{IQE}_{\text{particles}} / \text{IQE}_{\text{bare solar cell}}$ and $g(\lambda) = \text{IQE}_{\text{particles}}(\lambda) / \text{IQE}_{\text{bare solar cell}}(\lambda)$. The all electron-hole pair gives the photocurrent, so the short circuit current density $J_{sc}$ is defined as $J_{sc} = e \int \frac{A}{h_c} QE(\lambda) I_{AM1.5}(\lambda) \mathrm{d}\lambda$, where $e$ is the electron charge. For DEVICE, efficiency is defined as $\eta = (\text{FF} \times V_{oc} \times J_{sc})/S_{AM1.5G}$, where $FF$ is the fill factor, $V_{oc}$ is the open-circuit voltage, $J_{sc}$ is the short-circuit current, and $S_{AM1.5G}$ is the incident power from the AM1.5G solar model, which is equal to 100mW/cm$^2$. The fill factor is related to the maximum power point, where $JV$ is the maximum value, and FF is defined as $\text{FF} = P_{max} / V_{oc}$. $J_{sc}$ and the efficiency $\eta = P_{max} / S_{AM1.5G}$.

3.7.2 Computer Model

In this study, the c-Si/a-Si:H/µc-SiGe tandem solar cell is designed by staking the sub-cell with band gaps 1.12, 1.5, and 1.7 eV respectively. The graphical user interface (CAD) of design is shown in Figure 3.4. The total generation rate optical efficiency, for two different polarized and un-polarized sources, is calculated in FDTD solution. Data for amorphous silicon, the index values $(n = n + ki)$, is used from the sources (Basore & Clugston, 2003; Software Spectra) and for µc-Si$_{0.85}$Ge$_{0.15}$, index values $(n = n + ki)$ are used from IOFFE Institute (IOFFE). These calculated photo generation rates are transported into DEVICE to achieve electrical efficiency and power conversion efficiency. A fixed amount of trap density for amorphous silicon $(N_{t_e} = 7e18$ and $N_{t_h} = 5e17$) and capture cross section per cm$^2$ $(\sigma_e = 1e16$ and $\sigma_e = 1e16$ and $\sigma_h = 1e15$) are adjusted to calculate the carrier RSH recombination lifetime with Fossum life time correction model, in Lumerical FDTD / Device 4.6 (Solutions FDTD, 2016). In
addition to these calculations, three different models from sources (Abdul-Hadi, Hashemi, DiLello, Polyzoeva, Nayfeh, & Hoyt, 2013; Nelson, 2003; Hvam & Brodsky, 1981; and Schenk, 1992) were studied and the most suitable parameter values for the c-Si/a-Si:H/µc-SiGe tandem solar cell were extracted. These values are given in Table 3.1.

The solar cell is designed in two steps. First, the optical characterization of material is performed in FDTD and then it is transported into DEVICE for electrical characterization. Within DEVICE, the effective lifetime $\tau_{\text{eff}}$ of µc Si:H, a-Si:H and µc-SiGe layers are extracted from the measured solar cell parameters (Solutions FDTD, 2016; Abdul-Hadi, Hashemi, DiLello, Polyzoeva, Nayfeh, & Hoyt, 2013; Nelson, 2003). According to Hadi, et al. (Abdul-Hadi, Hashemi, DiLello, Polyzoeva, Nayfeh, & Hoyt, 2013), the open circuit voltage for a solar cell is defined as $V_{\text{oc}} = \frac{kT}{q} \ln \frac{J_{\text{ph}}}{J_{\text{dark}}}$ where $J_{\text{ph}}$ is the total generated photon current and
Table 3.1: Important parameters and structural dimensions used in this simulation

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>c-Si layer</th>
<th>μc-Si(i) layers</th>
<th>a-SiH layer</th>
<th>μ-SiGe layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer thickness (µm)</td>
<td>0.30</td>
<td>0.10</td>
<td>1.20</td>
<td>1.50</td>
</tr>
<tr>
<td>Band gap, Eg (eV)</td>
<td>1.12</td>
<td>1.12</td>
<td>1.50</td>
<td>1.70</td>
</tr>
<tr>
<td>dc permittivity</td>
<td>11.70</td>
<td>11.70</td>
<td>11.90</td>
<td>12.20</td>
</tr>
<tr>
<td>(n_i) (1/cm(^2))</td>
<td>1.05×10(^{10})</td>
<td>1.39×10(^{10})</td>
<td>6.10×10(^6)</td>
<td>127471</td>
</tr>
<tr>
<td>Work function (eV)</td>
<td>4.20</td>
<td>4.20</td>
<td>4.20</td>
<td>4.20</td>
</tr>
<tr>
<td>Electron mobility (cm(^2) V(^{-1}) s(^{-1}))</td>
<td>1471.00</td>
<td>1471.00</td>
<td>1471.00</td>
<td>1471.00</td>
</tr>
<tr>
<td>Hole mobility (cm(^2) V(^{-1}) s(^{-1}))</td>
<td>470.50</td>
<td>470.00</td>
<td>470.00</td>
<td>470.00</td>
</tr>
<tr>
<td>SRH life time for e (s)</td>
<td>3.30×10(^{-6})</td>
<td>1.00×10(^{-10})</td>
<td>1.20×10(^{-12})</td>
<td>1.20×10(^{-11})</td>
</tr>
<tr>
<td>SRH life time for h (s)</td>
<td>4.00×10(^{-6})</td>
<td>1.00×10(^{-10})</td>
<td>0.70×10(^{-12})</td>
<td>0.70×10(^{-11})</td>
</tr>
<tr>
<td>Radiative life time for e/h (s)</td>
<td>1.60×10(^{-14})</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Auger life time for e (s)</td>
<td>2.80×10(^{-31})</td>
<td>2.80×10(^{-31})</td>
<td>2.80×10(^{-31})</td>
<td>2.80×10(^{-31})</td>
</tr>
<tr>
<td>Auger life time for h (s)</td>
<td>9.90×10(^{-32})</td>
<td>9.90×10(^{-32})</td>
<td>9.90×10(^{-32})</td>
<td>9.90×10(^{-32})</td>
</tr>
<tr>
<td>Interface recombination velocity (cm/s)</td>
<td>1.00×10(^7)</td>
<td>1.00×10(^8)</td>
<td>1.00×10(^{10})</td>
<td>1.00×10(^{10})</td>
</tr>
</tbody>
</table>

\(J_{dark}\) is dark current. The \(J_{dark}\) dark current can be further expressed as: 

\[
J_{dark} = q \frac{L_{np}}{\tau} \frac{n_i^2}{N_{A,D}}
\]

From these equations, we can finally derive the lifetime for the carrier in terms of trap-assisted SRH recombination, which is given as:

\[
\tau = q \frac{n_i^2 L_{np}}{N_{A,D} J_{ph}} e^{\frac{V_{oc}}{kT}}
\]

According to Lumerical model (Solutions FDTD, 2016) the lifetime in terms of trap-assisted SRH recombination is:

\[
\tau_{eff} = (N_t \sigma \sqrt{\frac{3k_B T}{m^*}})^{-1}
\]

where \(N_t\) is trap density and \(\sigma\) is the capture cross-section per cm\(^2\). The carrier lifetime of a high quality bulk Si wafer is typically in the 1 ms range. The Si epi layer lifetime, it is typically around 100 µs (Park, Schroder, Tan, ChoiFletcher, Buczkowski, & Kirscht, 2001). Similarly, for the SiGe layer, the lifetime is reported to be lower, in the range 30 to 40 µs with an impurity doping.
concentration $10^{17}$ to $10^{19}$ cm$^{-3}$ depending on the growth technique (Chakraborty, Bera, Bhattacharya, Bose, & Maiti, 2006).
CHAPTER 4

Results and Discussion for One-Dimensional Analysis
4.1 Model Design and Parameters

The simulation of an amorphous silicon heterojunction solar cell is performed by using AFORT-HET (Stangl, Leendertz, & Haschke, 2010). The schematic layout and software provided layer structures are shown in Figure 4.1.

(a) Structural design in AFORS-HET-2.4.1 (b) Schematic layout.

For simulation of any device, structure identification of the basic device parameters is very important. These parameters have a great influence on its electrical and optical properties as well as on the overall device performance. All its performance, behavior, and output depend on its input parameters. In designing an amorphous silicon (a-Si) heterojunction solar cell, the important parameters are the band gap, thickness, and defective density of states (donor-like and accepter-like states) in absorbing layer and at interfaces. Temperature, career concentration, and
mobility parameters are also influencing factors in the case of an a-Si solar cell. Figure 4.1 shows (a) the device layers designed in AFORS-HET and (b) the schematic layout of its structure.

An n-type 80nm indium doped tin oxide (ITO) layer is used at the top surface. The selection of ITO is because of its high transparency, low series resistance, and minimum optical losses for the useful spectral range. A 20 nm thick layer of Ag is used as the bottom layer. For both the ITO and bottom layer Ag, the default optical constant models (n(E) and k(E)) are available in the database of AFORS-HET software (Stangl, Leendertz, & Haschke, 2010). Simulations are performed for both absorbing layers a-Si:H and a-SiGe:H, first separately, and then they are combined in a tandem structure (a-Si:H+a-SiGe:H). In all simulations, including a-Si:H, a-SiGe:H, and in the tandem structure, a wide band gap (1.85eV) thin intrinsic a-SiC is used as the window layer. This layer helps to reduce the interface recombination and improves the interface quality with better surface passivation. Using the same concept, two buffer layers (intrinsic silicon layers, layer 5 and layer 7) are inserted at interfaces, a-Si:H/a-SiGe:H and a-SiGe:H/a-Si(n), as shown in Figure 4.1.

Introducing such buffer layers helps to improve the Voc of the cell. The band gap of these intrinsic silicon layers, layer 5 and layer 7, is 1.7eV. The intrinsic silicon a-Si(i) layer 7 acts as the back surface field layer and we will analyze its blocking effect, which is the reduction of the recombination of minority carriers during drift towards the wrong contact. The a-Si:H, having a 100nm thickness with graded band structure, is considered to be the main absorbing layer in the device. The energy band gap of this layer varies from 1.75 eV at the top to 1.65eV at the bottom. The second main absorbing layer, a-SiGe:H, having a thickness of 80nm with a fixed band gap of 1.55eV, is used. The complete band gap diagram of the device is shown in Figure 4.2.

To design a p-i-n model, an a-Si p-type layer at the top (with a thickness of 5 nm and Na = 3e18 cm\(^{-3}\)) and an a-Si n-type layer at the bottom (with Nd = 8e18
cm\(^3\) with a thickness of 5nm) is used to separate the photo-generated carriers with the help of a reverse field. These layers provide drift to photo generated electrons and holes in the intrinsic region and help to collect them at the respective terminal. The band gap of the top layer of a-Si (p\(^+\)) is 2eV and the bottom n-type layer a-Si (n\(^+\)) is 1.8eV.

**Figure 4.2** Band diagram of the device (a) without and (b) with notation of layers and holes in the intrinsic region and help to collect them at the respective terminal.
Simulation results always rely on the physical model and model parameters. To perform simulation and to obtain the desired results, a proper physical model and model parameters must be used as initial values. Usually initial parameters are selected from the experimental data. For this study, all parameters for all layers (a-SiC, a-Si(i), a-Si:H, and a-SiGe:H) are selected from the previous literature (Nelson, 2003; Shaoying, Chong, Tao, Jie, & Yu, 2014; Saito, Li, Ikeda, & Shirai, 2006; Uesugi, Ihara, & Matsumura, 1985; Schmid & Seidel, 2006; Mokeddem, Aoucher, & Smail, 2006; and Sai, Matsui, Matsubara, Kondo, & Yoshida, 2014) and optimized during the design with AFORS-HET. These parameters are given in Table 4.1.

Disordered materials such as a-Si:H, a-SiGe:H and a-SiC:H contain a large number of defect states within the band gap. To accurately model the device, we consider the continuous density of defect states in a-Si and in all of its alloys. The Density of States (DOS) is described as a combination of exponential decaying band tail states (for both donor-like states and acceptor-like states) and Gaussian distribution of mid-gap states as shown in Figure 4.3. The a-Si:H characteristic energies of conduction band and valance band tails are 0.06 eV and 0.03 eV. Similarly, the peak energy distributions of acceptor- and donor-type Gaussian states are 1.2 eV and 0.56 eV with a deviation of 0.08 eV. The concept of a Gaussian distribution of defect states in an amorphous silicon material reflects its disordered structure and the disorder of states rather than its location at a particular energy level. This distribution of density of defect states is designed for all layers including a-SiC and a-Si(i) layers. The layers a-SiC and a-Si(i) are very thin, so the high defect density in these buffer layers does not affect the efficiency of the solar cell too much.

The physical model of the device describes the operational phenomena while model parameters are calibrated to the procedure and selected materials are used to fabricate the device. AFORS-HET solves Poisson’s equation and two career continuity equations by finite differences and the Newton-Raphson technique under the equilibrium and nonequilibrium steady state conditions. At the first stage, a-Si
Table 4.1 Important Parameters and Structural Dimensions Used In This Simulation

<table>
<thead>
<tr>
<th>Parameter Name</th>
<th>a-SiC layer</th>
<th>a-Si(i) layers</th>
<th>a-SiH layer</th>
<th>a-SiGe:H layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layer thickness (nm)</td>
<td>10.00</td>
<td>10.0/20.0</td>
<td>100.00</td>
<td>80.00</td>
</tr>
<tr>
<td>Band gap, Eg (eV)</td>
<td>1.85</td>
<td>1.7</td>
<td>1.75-1.65</td>
<td>1.55</td>
</tr>
<tr>
<td>Electron affinity (eV)</td>
<td>4.03</td>
<td>3.9</td>
<td>3.95</td>
<td>4.17</td>
</tr>
<tr>
<td>Effective conduction band density (cm⁻³)</td>
<td>2.846e19</td>
<td>1e20</td>
<td>2.5e20</td>
<td>2.846e19</td>
</tr>
<tr>
<td>Effective valence band density (cm⁻³)</td>
<td>2.846e19</td>
<td>1e20</td>
<td>2.5e20</td>
<td>2.846e19</td>
</tr>
<tr>
<td>Electron Mobility (cm³ V⁻¹ s⁻¹)</td>
<td>20.00</td>
<td>20.00</td>
<td>20.00</td>
<td>20.00</td>
</tr>
<tr>
<td>Hole Mobility (cm³ V⁻¹ s⁻¹)</td>
<td>2.00</td>
<td>5.00</td>
<td>2.00</td>
<td>2.00</td>
</tr>
<tr>
<td>Total DOS in acceptor like Gaussian (cm⁻³)</td>
<td>5e17</td>
<td>5e17</td>
<td>5e17</td>
<td>5e17</td>
</tr>
<tr>
<td>Total DOS in donor like Gaussian (cm⁻³)</td>
<td>7e15-5e17</td>
<td>5e17</td>
<td>7e15-5e17</td>
<td>5e17</td>
</tr>
<tr>
<td>Gaussian donor like peak energy (eV) from Ec</td>
<td>1.2</td>
<td>1.12</td>
<td>1.2</td>
<td>1.12</td>
</tr>
<tr>
<td>Gaussian acceptor like peak energy (eV) from Ev</td>
<td>0.7</td>
<td>0.56</td>
<td>0.56</td>
<td>0.6</td>
</tr>
<tr>
<td>Standard deviation (eV)</td>
<td>0.08</td>
<td>0.08</td>
<td>0.08</td>
<td>0.08</td>
</tr>
<tr>
<td>Capture cross-section for donor states e, h (cm³)</td>
<td>1e-15, 1e16</td>
<td>1e-15, 1e16</td>
<td>1e-15, 1e16</td>
<td>1e-15, 1e16</td>
</tr>
<tr>
<td>Capture cross-section for acceptor states e, h (cm³)</td>
<td>1e-17, 1e15</td>
<td>1e-17, 1e15</td>
<td>1e-17, 1e15</td>
<td>1e-17, 1e15</td>
</tr>
<tr>
<td>Characteristic energy for donor and acceptor (eV)</td>
<td>0.06 0.3</td>
<td>0.055 0.03</td>
<td>0.06 0.3</td>
<td>0.06 0.3</td>
</tr>
<tr>
<td>Donor concentration (cm⁻³)</td>
<td>0.00</td>
<td>1000.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Acceptor concentration (cm⁻³)</td>
<td>0.00</td>
<td>1e7</td>
<td>1e7</td>
<td>1e7</td>
</tr>
<tr>
<td>Electron and hole thermal velocity (cm/s)</td>
<td>1e7</td>
<td>1e7</td>
<td>1e7</td>
<td>1e7</td>
</tr>
<tr>
<td>Layer density (g.cm⁻³)</td>
<td>2.328</td>
<td>2.328</td>
<td>2.328</td>
<td>2.328</td>
</tr>
</tbody>
</table>

alloyed layers are selected for the specified purpose and then the device is modeled by specifying corresponding layers and its interface properties, i.e., the defect distribution of states (DOS) shown in Figure 4.3. Using Shockley-Read Hall recombination statistics, one-dimensional equations are solved for thermodynamic equilibrium for steady-state conditions by applying external voltage or current, with illumination (AM1.5 radiation).
Current-voltage (IV) characteristics and internal and external quantum efficiency (QE) are investigated by changing a variety of input parameters for each layer. For front and back contacts, the MS Shockley model is applied. The drift diffusion model and thermionic emission model are used for the interfaces. The Labert-Beer absorption model is applied for the optical bulk layer.

Figure 4.3 Defect density distribution of conduction and valance band tail states and two Gaussian states for hydrogenated (a) a-Si:H and (b) a-SiGe:H
4.2 Dark Characteristics

The dark characteristics of the device (before applying an external voltage), the band gap diagram, charge carrier concentration, current density, and generation rate are shown in Figure 4.4.

Figure 4.4 Dark characteristics before applying external voltage:
(a) band diagram, (b) current density holes and electrons, (c) charge carrier concentration, and (d) total current density.

The results in the graph represent the electron and hole current density at the edges of blocking layers. a-SiC acts as a blocking layer for the electrons due to the band gap difference, and according to the band structure, the holes are likely to move towards the p-type top layer. On the other end, the a-Si(i) n’ layer blocks
minority carriers towards the n-type bottom layer while the band gap structure supports electrons to move towards it. Both layers act as blocking layers for electrons and holes at their interfaces with the bulk absorption layers; therefore, the current density is high at these points, as shown in Figure 4.4 graph (d). There is no external voltage and no light applied externally so there is no generation current. The charge carrier concentration is shown near the p-type top layer and n-type bottom layer in graph (c).

After applying external voltage and reverse biasing the solar cell, the band bending is as shown in Figure 4.5 (a).

**Figure 4.5** Characteristic graphs after applying an external voltage of -1.5v: (a) Bending of band diagram with application of external voltage, (b) Generation and recombination (c) Current density, and (d) Charge carrier concentration
4.3 Light IV Characteristics

The default illumination source provided by the software is AM 1.5 radiations with a power density of 100mW/cm². Light was applied externally to the device in reverse bias, with -1.5V. The IV characteristics are demonstrated as shown in Figure 4.6 (a).

\[
V_{oc}=1.045 \text{ mV} \quad J_{sc}=11.66 \text{ mA/cm}^2 \quad FF=85.95 \% \quad Eff=10.46 \%
\]

(a)

Figure 4.6 Light characteristics (a) IV, (b) hole concentration, and (c) electron concentration

The electron and hole recombination is increased as compared to the dark conditions due to an increase in the total regeneration of electrons and holes (due to
both photo generation and thermal generation). The temperature was kept constant for this procedure at 300K. Total recombination of electrons and holes increases at the interface between a-Si:H and the intrinsic buffer layer a-Si(i). The overall conversion efficiency of the device is 10.46% with Voc = 1045 mV, Jsc = 11.66 mA/cm² and Fill factor, FF = 85.85%.

4.4 Spectral Absorption: Internal and External Quantum Efficiency

Quantum efficiency helps describe the spectral response of the device with respect to the wavelength. The external quantum efficiency (EQE) of the device is shown in Figure 4.7.

![Incident spectrum](image1.png)

(a) Incident spectrum.

![Spectral response](image2.png)

(b) Spectral response.

**Figure 4.7** (a) Incident spectrum. (b) Spectral response
The internal quantum efficiency goes to zero when an incident photon has an energy value less than the band gap. This phenomenon is observed for a value above the wavelength 800nm. Internal quantum efficiency should be always greater than the external quantum efficiency since the IQE governs the generation of electrons by absorption of each photon. The external efficiency depends on both the absorption and collection of charges. In Table 4.2, we can compare the external quantum efficiency with internal quantum efficiency (IQE).

**Table 4.2 Values of IQE and EQE**

<table>
<thead>
<tr>
<th>S. No</th>
<th>lambda (nm)</th>
<th>IQE Tandem</th>
<th>EQE Tandem</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>300</td>
<td>8.867e-1</td>
<td>8.938e-1</td>
</tr>
<tr>
<td>2</td>
<td>366</td>
<td>9.358e-1</td>
<td>9.385e-1</td>
</tr>
<tr>
<td>3</td>
<td>433</td>
<td>9.649e-1</td>
<td>9.623e-1</td>
</tr>
<tr>
<td>4</td>
<td>500</td>
<td>9.811e-1</td>
<td>8.823e-1</td>
</tr>
<tr>
<td>5</td>
<td>566</td>
<td>9.846e-1</td>
<td>5.503e-1</td>
</tr>
<tr>
<td>6</td>
<td>633</td>
<td>9.921e-1</td>
<td>2.051e-1</td>
</tr>
<tr>
<td>7</td>
<td>700</td>
<td>9.999e-1</td>
<td>3.245e-2</td>
</tr>
<tr>
<td>8</td>
<td>766</td>
<td>9.999e-1</td>
<td>9.136e-3</td>
</tr>
<tr>
<td>9</td>
<td>833</td>
<td>0.000e+0</td>
<td>1.510e-7</td>
</tr>
</tbody>
</table>
4.5 Variation in Efficiency with Change in Band Gap and Thickness

The efficiency of the solar cell depends upon the band gap of the absorbing layer. We changed the band gap of a-Si:H from 1.65eV to 1.75eV and investigated the change in efficiency as a function of the band gap, as shown in Figure 4.8. The efficiency reaches its maximum value 10.46% in the range of 1.71 to 1.725 eV. Fill factor FF reaches a maximum of 85.5 near 1.7ev. Increasing the absorber thickness increases the open circuit voltage and simultaneously decreases the short circuit current of the solar cell. The efficiency of the solar cell as investigated by varying the thickness of the a-SiH layer from 50nm to 110nm. The values maximize the efficiency at 120nm, but it starts to reduce FF above from 110nm, as shown in Figure 4.9.

Figure 4.8 Change in efficiency with respect to change in the band gap of the a-Si:H layer.
The fill factor has the highest value at the thickness between 95nm and 105nm. The efficiency of the cell increases with increasing thickness as expected due to the increase in Voc and decrease in Jsc but the FF is increased.

Similarly, the efficiency of the solar cell is investigated by varying the band gap of the a-SiGe:H second absorber layer from 1.45 eV to 1.55 eV. The efficiency decreases with a decrease in band gap, similar to that before, but we tried here to optimize the efficiency for a-SiGe:H too. The thickness of the same layer was also varied and the efficiency was observed to optimize the values. The output graphs are shown in Figure 4.10 (a), (b), and (c) for the a-SiGe:H layer. At a thickness greater than 90nm thickness in a-SiGe:H, the recombination of electrons and holes increases very rapidly due to the Staebler-Wronski effect (Chang, Lu, Yeh, & Houng, 2012). As a result of significant degradation of the electric field inside the layer, the fill factor and efficiency goes down.

![Figure 4.9](image)

**Figure 4.9** Efficiency (a) and FF (b) with respect to change in thickness of the a-Si:H layer
Figure 4.10  Efficiency response: (a) Efficiency vs. band gap variation of the a-SiGe:H layer; (b) Efficiency vs. thickness and (c) FF vs. thickness of the a-SiGe:H layer
4.6 Effect of Temperature

In a-Si-based solar cells, both the conversion efficiency and the light induced degradation were challenging to control from the beginning of the solar research. The defect density of hydrogenated amorphous silicon (a-Si:H) increases with light exposure, which causes an increase in recombination of electrons and holes through defect states. As a result, the conversion efficiency reduces. This particular nature of the effect was known as the Staebler Wronski effect. It was proposed that the electron hole pair formed by incident light may break the neighboring bonds, which again causes recombination of these carriers. Moreover, there always exist free hydrogen atoms in a-Si:H, which produce dangling bonds at high temperature and these dangling bonds are the sources of defect states in a-Si:H. In this design, the a-SiGe:H layer is introduced with the purpose to maintain the reliability against light soaking. In the a-SiGe:H, the efficiency is controlled for a certain period of time and at high temperature.

![Graphs showing change in Fill factor and efficiency with respect to change in temperature from 300K to 400K.](image)

(a) FF (T) | (b) Eff (T)

**Figure 4.11** Change in Fill factor and efficiency with respect to change in temperature from 300K to 400K

From Figure 4.11, it is clear that the variation in efficiency is from 10.46% at 300K to 7.56% at 400K, which is really not so poor. The increase in temperature for both
Voc and Jsc increases, but the net recombination of charge carriers reduces the fill factors and efficiency.

4.7 Effect of Back Surface Field (BSF)

The back-surface field referred to the layer, acts like a barrier for minority carriers, thereby, reducing the recombination photo-generated carriers in the back surface region. This layer usually contributes not only to increasing photo-generated current but also increases photo voltage. In the design, intrinsic amorphous silicon is used as BSF with a thickness of 20 nm. The Voc varies from -1.045 to -1.0468eV, Joc increases, FF reduces, and the overall conversion efficiency of the layer increases with increasing the thickness of the BSF layer. The J-V characteristic is shown in Figure 4.12.

**Figure 4.12** Change in Fill factor and efficiency with respect to change in thickness of the BSF layer
The effect is also investigated at high doping concentration. In Table 4.3, it is shown that the effect of the BSF doping density improves the efficiency of the device. The efficiency increases with an increase in concentration until it reaches $1.0526 \times 10^{20} \text{ cm}^3$, and then a drastic reduction is shown. With the increasing doping concentration, the short circuit current, open circuit voltage, and fill factor are increased, but the Voc saturates at near $5.2633 \times 10^{19} \text{ cm}^3$ as a result of degeneracy.

Table 4.3 Variation in efficiency due to change in doping density of the BSF layer

<table>
<thead>
<tr>
<th>S.No</th>
<th>Nd (cm$^{-3}$)</th>
<th>Voc (V)</th>
<th>$J_{sc}$ (A/cm$^2$)</th>
<th>FF</th>
<th>Eff</th>
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<td>-1.1429E-2</td>
<td>8.5143E-1</td>
<td>1.0197E-1</td>
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</table>

The effect due to change in band gap was also investigated as the band gap varied from 1.2 to 1.8eV. The Voc voltages initially increase and then saturate at about 1.53eV. The fill factor decreases after 1.4eV and leads to a decrease in conversion efficiency after 1.66eV. As the band gap broadens, it interferes as a barrier for the majority carriers too. The optimum band gap selected for the BSF layer is 1.5-1.7 eV. The results are shown in Table 4.4.
Table 4.3 *Variation in efficiency due to change in band gap of the BSF layer*

<table>
<thead>
<tr>
<th>S.No</th>
<th>Eg (eV)</th>
<th>Voc (V)</th>
<th>Jsc (A/cm^2)</th>
<th>FF</th>
<th>Eff</th>
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<td>9.6583E-2</td>
</tr>
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<td>-1.0442</td>
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<td>1.0146E-1</td>
</tr>
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<td>-1.1398E-2</td>
<td>8.5135E-1</td>
<td>1.0168E-1</td>
</tr>
</tbody>
</table>

4.8 Effect of the Variation in the Thickness Of Buffer Layers

The effect of the thickness is shown in Figure 4.13. The thicknesses of the buffer layers of a-Si(i) varied from 5nm to 15nm. The Voc decreases, current increases, and FF and efficiency also increase with the increasing thinness of the a-Si(i) buffer layers. The overall efficiency increases from 10.18 to 10.29%. We consider a 10nm thinness for these buffer layers as the optimum thickness value. Keeping all the conditions the same except eliminating the buffer layers, the efficiency reduces to 9.71% with Voc = 1049mA, Joc = 10.83mA/cm^2, and with Fill factor, FF = 85.56%.
Figure 4.13 Variation in overall efficiency with the thickness of buffer layers

4.9 Role of Tunneling

The thermionic emission model is used for Space Charge Limited Current (SPLC) (Nelson, 2003) and for the recombination current across the interface. The transfer of the charge carrier from one side to the other side across the interface is modeled via thermionic emission and recombination of defect states. These defect states not only interact with one another but also interfere the transport from one semiconductor to another semiconductor by adjacent interaction. As a result, the distribution function of the defect states is modeled by the four capture cross-sections; for electrons $\sigma_{n1} = 1 \times 10^{-17}$ cm$^2$ and $\sigma_{n2} = 1 \times 10^{-16}$ cm$^2$; for holes $\sigma_{p1} = 1 \times 10^{-15}$ cm$^2$ and $\sigma_{p2} = 1 \times 10^{-15}$ cm$^2$ (two for holes and electrons each for two joining semiconductors). The potential is assumed to be continued across the interface, unlike the buffer layer acting like a dipole.
We took the earlier work on the transport at the hetero-interface on solar cell performance (Keppner, Meier, Torres, Fischer, & Shah, 1999) and applied it to interface 2 and interface 5. The default values of the Richardson constant for the electron and holes were $A_e$ and $A_h = 9.56186 \text{ As/cm}^2\text{K}^2$ for a-SiC and a-Si chosen from the software. From the selection of interfaces for the thermionic emission model, it was obvious that interface 2 blocks the holes and interface 5 blocks the electrons due to abrupt interfaces. Most likely, tunneling happens across these two interfaces. The efficiency of the device is compared with and without tunneling. With tunneling, the efficiency is reduced to 10.18 percent with $V_{oc} = 1047\text{mV}$, $J_{sc} = -11.48\text{mA/cm}^2$, and $FF = 84.75$ percent. The results are shown in Figure 4.14; the carrier charge concentration reduces at these two interfaces compared to that without tunneling results. Moreover, the band gap of the a-SiGeH is varied from 1.4 to 1.55 eV to assess the interface effect at interface 5. The efficiency reduces for the smaller band gap values due to the larger conduction band off; as a result, a few electrons can surmount the barrier. Although tunneling is critical in modeling semiconductor devices for getting a reliable performance.

**Figure 4.14** Charge carrier concentration at the interfaces
over a wide range of discontinuities, its effect usually decreases the efficiency for a large band of values.

4.10 Influence of Defect Density

Amorphous silicon (a-Si:H) possesses the disorder or short-range order of atoms that gives rise to a definite band structure; having mobility edges treated as conduction and valance band edges defines the mobility gap. The energy states in the band gap act as trapping and recombination centers that affect the device performance. The charge carrier lying in the band tails and dangling bond defect states do not contribute to conduction at normal temperature. Making alloys of a-Si:H increases the density of the dangling bonds by widening the conduction band tail. All these changes affect the charge carrier mobility and trapping and recombination lifetime. The effect of defect density for both absorbing layers (a-Si:H and a-SiGe:H) has been studied. Generally, the increase in the defect density of states causes a reduction in efficiency. Figure 4.15 shows the response of the variation in defect density of the a-Si:H absorbing layer versus efficiency of the device from $7 \times 10^{12} \text{ cm}^{-3}$ to $7 \times 10^{18} \text{ cm}^{-3}$. These results show that the drop in efficiency rate is fast at lower density of states. As the density of states increases from $1 \times 10^{18} \text{ cm}^{-2}$, the rate in change in efficiencies becomes slower and smoother. This is because the density of states is more effective in degradation of performance from $1 \times 10^{12} \text{ cm}^{-3}$ to $1 \times 10^{17} \text{ cm}^{-3}$; after $1 \times 10^{17} \text{ cm}^{-3}$, efficiency is so reduced that its change in rate is very minor and smoothed.

These simulated results do not reflect the previous literature where the efficiency is approximately constant (Yang, Yan, & Guha, 2005; Solutions FDTD, 2016) up to $1 \times 10^7 \text{ cm}^{-3}$ and then starts decreasing for further reduction in defect density. The efficiency rapidly reduces at higher density of states (Shaoying, Chong, Tao, Jie, & Yu, 2014) beyond $1 \times 10^7 \text{ cm}^{-3}$ as compared to lower density of states. The difference in results is due to the thickness of thin film (80 to 110 nm), while previous results were investigated for 5nm.
Figure 4.15 The effect of defect density of states, at the a-Si:H layer, on the efficiency of the device.

Figure 4.16 The effect of the defect density of states on the efficiency of the device a-SiGe:H.
4.11 Interface Properties

Regarding a-Si:H, one of most challenging jobs is to design the interface while keeping the density of interface states and defects as low as possible to prevent recombination losses. With this point of view, the sensitivity of recombination velocity affecting the performance of the device was studied. The recombination velocity is varied from 10 to 1x10⁷ cm/s. The rate of change in efficiency is very rapid from 1x10⁴ cm/s to 1.5 x10⁶ cm/s as shown in Figure 4.17. At a fixed value of recombination velocity equal to 1.5 x10⁶ cm/s, the efficiency reduces to 9.76 % with Voc = -1046.2 mV, Joc = -11.51 mA/cm², and FF = 81.13%.

![Figure 4.17 Effect of recombination velocity on the efficiency at interface](image)

To assess the interface properties a certain number of defect densities at fixed locations in the interface between two semiconductors are inserted. Interface 2 and interface 5 are selected for the defect densities. These trap centers, whose associated energy lies in the forbidden gap, exchange charge with the conduction and valance band through the emission and capture of charge particles. After
inserting a fix number of defect density \((1 \times 10^{12} \text{ cm}^{-2})\) with capture cross-sections of electrons \(\sigma_{n1} = 1 \times 10^{-17} \text{ cm}^2\) and \(\sigma_{n2} = 1 \times 10^{-16} \text{ cm}^2\), for holes \(\sigma_{p1} = 1 \times 10^{-15} \text{ cm}^2\) and \(\sigma_{p2} = 1 \times 10^{-15} \text{ cm}^2\), the efficiency reduces to 5.972 % with \(V_{oc} = -994.2 \text{ mV}\), \(J_{oc} = -7.189 \text{ mA/cm}^2\), and \(FF = 83.56\%\). Usually, inserting a fixed value of defect density greater than \(1 \times 10^{12} \text{ cm}^{-3}\) causes the response of the device to become irregular and hard to assess. The reduction in efficiency is due to the reduction in \(V_{oc}\) by recombination at the interfaces.

![Graph](image)

**Figure 4.18** Effect of defect density of states on the efficiency at the interface

The trap density behavior, presented here in Figure 4.18, is qualitatively similar to the previous literature (Nawaz, 2011). For a given band offset, at a particular location of interface, drops in efficiency with varying interface defect state density from \(1 \times 10^9 \text{ cm}^{-3}\) to \(1 \times 10^{12} \text{ cm}^{-3}\) have been obtained.

### 4.12 Investigating the Individual Absorbing Layer a-Si:H AND a-SiGe:H

In addition to analyzing the tandem design, both individual layers are investigated as single absorbing layers. For both device structures, the schematic designs are shown in Figure 4.19. The a-Si:H schematic layer designs are shown in
part (a) and a-SiGeH shown in (b). The efficiencies of both designs are compared with the tandem design. Figure 4.20 shows the efficiencies (IV characteristic) of a-Si:H, a-SiGe:H, and tandem (a-Si:H+a-SiGe:H) cell.

![Schematic diagram of individual layers a-Si (a) and a-SiGeH (b)](image)

**Figure 4.19** Schematic diagram of individual layers a-Si (a) and a-SiGeH (b)

As mentioned above, the tandem cell efficiency is 10.46%. The efficiency of the a-Si:H individual layer is 9.638% with FF = 83.07%, Voc = 1069mV, and Jsc = 10.86 mA/cm². The Voc is highest compared to the other designs due to the thickness of the layer. The short circuit current is nearly comparable to the tandem design. It is because of the high band gap of a-Si:H compared to a-SiGeH. The a-Si:H layer is sensitive to thermal generation; there is higher generation rate as compared to other layers, but it has high recombination. The efficiency of a-SiGe:H is about 5.398% with FF = 81.85%, Voc = 1026mV, and Jsc = 6.429 mA/cm². Obviously, the short circuit current and efficiency of a-SiGe:H is lower because of lower band gap and thickness, but it has high reliability as compared to a-Si:H by having less defect density.
Figure 4.20  Comparison of efficiencies (a) Green line: a-Si:H, (b) Red line: a-SiGe:H, and (c) Blue Line: tandem design (a-Si:H + aSiGe:H).

4.13 Spectral Response of Each Layer

We can compare the external quantum efficiency with the internal quantum efficiency of each layer. The internal quantum efficiency goes to zero when the incident photon has energy less than the band gap. This is what we observed at a wavelength of 766nm. The least absorbing layer is obviously a-SiGe:H, while with a combination of both individual absorbing layers, a little increase in the QE is observed. The QE of a-SiC is also assessed, but due to very weak absorption coefficient, considering it as an absorber was ruled out. The spectral response of each layer is shown in Figure 4.21.
Figure 4.21 Spectral response of a-Si:H and a-SiGe:H as compared to tandem cell. (a) Green line: a-Si:H, (b) Red line: a-SiGeH, and (c) Blue Line: tandem design (a-Si:H + aSiGe:H).

Table 4.5 The internal (IQE) and external efficiencies (EQE) of a-Si: and a-SiGeH.

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<th>EQE a-Si:H</th>
<th>IQE a-SiGE:H</th>
<th>EQE a-SiGe:H</th>
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4.13 Conclusion

The numerical simulation of an amorphous silicon heterojunction thin film solar cell was performed by using AFORT-HET. The design of the tandem cell consists of a-SiC, a-Si:H, a-Si(i), and a-SiGe:H layers. a-SiC acts as a window and a-Si(i) acts as a buffer layer in the tandem design. a-Si:H and a-SiGe:H are the absorbing layers. Physical models and parameters used for the device simulation are mainly based on the device geometry and optimization of behavior. Dark and light characteristics, including contribution of each layer in increasing the efficiency, were analyzed. The dark current of $2.53 \times 10^{-8}$ mA cm$^{-3}$ at Voc =0V and at a temperature of 300K is recorded. The overall efficiency of the device is 10.46% with Voc = 1045 mV, Jsc = 11.66 mA/cm$^2$, and Fill factor, FF = 85.85% by applying AM 1.5 radiation (power density of 100mW/cm$^2$) at external voltage -1.5V. With the same conditions but without the buffer layer, the efficiency reduces to 9.71% with Voc = 1049mA, Joc = 10.83mA/cm$^2$, and with Fill factor, FF = 85.56%. The thickness of the buffer layer is optimized at 10nm with the defect density of $7 \times 10^{15}$ cm$^{-3}$. The spectral response of the device was assessed; simulation results show that internal quantum efficiency drops just after 766nm and external quantum efficiency is reduced after 800nm. The optimum efficiency for a-Si:H with band gap variation is achieved at 1.72 eV with -1.5V external voltage and 110 nm thickness. By changing the thickness at a fixed band gap of 0.55 eV, the response of a-SiGeH is optimized at 80nm. Simulation results regarding the effect of variation in temperature are observed. At 400K, the conversion efficiency of the device reduces to 7.65%. The 13nm thick a-Si(i) layer is used as the back surface field. The thickness of this layer is optimized up to 13nm and the band gap up to 1.5 to 1.7eV and with a doping density of $1.05 \times 10^{20}$ cm$^{-3}$. Observing the effect of defect density for both absorbing layers (a-Si:H and a-SiGe:H), the rate of the drop in efficiency is fast at lower density of states. As the density of states increases from $1 \times 10^{18}$ cm$^{-3}$, the rate in change in efficiencies becomes slower and smooth. It is due to the effect of the density of states, which are more effective from $1 \times 10^{12}$ cm$^{-3}$ to $1 \times 10^{17}$ cm$^{-3}$. 
By implementing tunneling through the interface via thermionic emission and recombination of defect states, the model is designed by the four capture cross-sections, two for the holes and two for the electrons for both the adjoining two semiconductors. The efficiency of the device is compared with and without tunneling. With tunneling, the efficiency is reduced to 10.18 percent. The recombination velocity at interfaces is varied from 10 to 1x10^7 cm/s and the rate of change in efficiency is noticed as it rapidly changes in between values 1x10^4 cm/s and 1.5 x10^6 cm/s. At a fixed value of recombination velocity at interfaces equal to 1.5 x10^6 cm/s, the efficiency reduces to 9.76 %. Moreover, simulating interface properties with a fixed number of defect densities (1 x 10^{12} cm^{-3}), capture cross-sections of electrons $\sigma_{n1} = 10^{-17}$ cm$^2$ and $\sigma_{n2} = 10^{-16}$ cm$^2$, capture cross-sections of holes $\sigma_{p1} = 10^{-15}$ cm$^2$ and $\sigma_{p2} = 10^{-15}$ cm$^2$, caused reduction in efficiency upto 5.972 %. The reduction in efficiency is due to the reduction in Voc by recombination at the interfaces.

Finally, each individual absorbing layer is assessed and the efficiency of the a-Si:H individual layer is 9.638% with FF = 83.07%, Voc = 1069mV, and Jsc = 10.86 mA/cm$^2$. The efficiency of a-SiGe:H is about 5.398% with FF = 81.85%, Voc = 1026mV, and Jsc = 6.429 mA/cm$^2$. 
CHAPTER 5

2D Computer Analysis and Optimization with Lumerical FDTD/DEVICE
5.1 Introduction

A thin film Si solar cell is considered to be an important and promising option in the solar industry as compared to the new generation photovoltaics. The cost of photovoltaic power remains relatively high due to the amount of silicon used in conventional wafer-based solar cells (Chang, Lu, Yeh, & Houng, 2012). The thin film solar cell was introduced due to its low cost and high flexibility, which permit installation on roofs or on any other non-uniform surface. The use of thin film technology in a solar cell greatly reduces the amount of pure silicon used as the active material. This together with easy processing and stability make it extremely suitable for mass production (Hamakawa, 2013; Nelson, 2003). Using amorphous and microcrystalline silicon in thin film technology is advantageous for low cost mass manufacturing, but it has serious light-induced degradation effects (C-W) after a long illumination time (Shaoying, Chong, Tao, Jie, & Yu, 2014).

Different methods are applied to resolve this C-W effect and to increase overall efficiency. When doping other atoms into silicon, such as Cl (Uesugi, Ihara, & Matsumura, 1985), F (Uesugi, Ihara, & Matsumura, 1985), C (Schmid & Seidel, 2006), and N (Mokeddem, Aoucher, & Smail, 2006) atoms into an a-Si:H thin film, these doped atoms break weak bonds and build stable bonds with doped atoms. A heat treatment process is also used to increase the diffusion of H in an a-Si:H cell (Yon, Astier, Bisotto, Chamingis, Durand, Martin, ... & Tissot, 2005). Among all the techniques the tandem design is mainly appreciated because it does not have a dominant C-W effect, especially in hydrogenated microcrystalline silicon. A tandem thin film design has lower bulk recombination (Hamakawa, 2013; Nelson, 2003) and the potential for increasing open circuit voltage if a high level of optical confinement can be achieved (Nelson, 2003). The hydrogenated amorphous silicon germanium (a-SiGe:H) is often used as an absorber layer material in a thin film solar cell to enhance the red response as compared to a-Si:H material (Nawaz & Ahmad, 2012). With the absorbing layer of a-Si:H, a-SiC is widely used as the window layer to increase optical transparency by widening the band of material.
Crystalline silicon is an indirect band gap and has a low absorption coefficient in the near infrared region. Thirty-six percent of photons have energies above the band gap of the Si wavelength region (Bermel, Luo, Zeng, Kimerling, & Joannopoulos, 2007); thus, the effective light confinement is essential to increase the overall efficacy of a tandem thin film solar cell. Recently, The Advanced Institute of Industrial Science and Technology (AIST) has designed a high efficiency (11.0%) microcrystalline silicon thin film solar cell using superior light trapping capability (honeycomb textured substrates) (Sai, Matsui, Matsubara, Kondo, & Yoshida, 2014). There are many ways to increase the photon absorption in the near IR region. Textured substrates have been developed (Berginski, Hüpkes, Reetz, Rech, & Wuttig, 2008) to scatter the incident light to increase the optical path inside the cells (Python, Madani, Dominé, Meillaud, Vallat-Sauvain, & Ballif, 2009) but it is noticed that the excessive steep texture substrate with a square-shaped or V-shaped valley often introduce defective porous areas and increasing light losses compared to its generation efficiency. This severely affects the device’s performance. In this study, the light trapping techniques are investigated and compared. The checkerboard, pyramidal structure, and quarter pyramid in empty checker light capturing techniques are designed. The efficiencies of these techniques are compared with the efficiency of a planner (without texture) solar cell and with anti-reflecting (AR) layers of ITO (TiO2) and Si3N4.

The tunneling junction is the core structure in a tandem solar cell. If the recombination in the tunneling process does not perform well, then this may damage the built-in potential at the interface and seriously affect device efficiency (Chang, Lu, Yeh, & Houng, 2012). The µc Si:H is regarded as a good choice for fabricating the tunnel junction due to its advantage of, for example, higher doping concentration, lower resistivity, and behavior ohmic contact (Yang, Yan, & Guha, 2005). A microcrystalline silicon layer with a band gap 1.12eV is used as the top interface layer between the a-Si:H middle layer with a band gap 1.5eV and the bottom layer µc-SiGe with a 1.7eV band gap. The purpose of creating this interface
layer is to investigate the effect of the tunneling process by inserting a very thin layer (0.1µm) of µc-Si:H between the middle and bottom layers.

The main objective of this study is to understand the challenges and improve the mechanism of efficiency degradation in microcrystalline and amorphous silicon tandem solar cells due to poor light confining techniques and recombination losses at the interface. The performance of a 2D thin film heterojunction solar cell is investigated with Lumeral FDTD/Device 4.6 (Solutions FDTD, 2016) and the efficiency is optimized.

5.2 Result and Discussion

5.2.1 Simulation of a Single Junction a-Si Solar cell

The two-dimensional numerical simulation of a single junction c-Si/a-Si layer is designed and implanted within Lumeral FDTD and DEVICE. The c-Si thin layer is used as the window layer and the a-Si layer is used as the main absorbing layer. The CAD view of a single layer a-Si is shown in Figure 5.1. The simulation is performed by considering the Schokley-Read-Hall recombination and Auger recombination models. Since the silicon is an indirect band gap material, the radiative recombination model is neglected. The trap-assisted lifetime is adjusted for electron and holes as 1.2e -12 s and 0.7e -12 s respectively in SRH recombination (Solutions FDTD, 2016; Nelson, 2003). For auger recombination, the capture coefficients for e = 2.8e-31 cm^4/s and for h = 9.9e-32 cm^4/s are adjusted, same as according to its default values for c-Si. According to the condition, considering only the generation rate and totally neglecting the recombination of carriers, the short circuit current J_sc in FDTD is noticed as 33.3012 mA/cm^2 and the total generation rate is 9.92911e+027 (1/m^2/s).

The device performance is evaluated and the efficiency of the design is optimized by varying the thickness of the main absorbing layer. To minimize the carrier recombination and other interface losses, highly doped p++ and highly
doped n++ regions are created at the emitter and at the base. For both the emitter and the base, Al is used as the contact metal. To enhance the absorption and maximize light trapping, a checkerboard surface is created. The c-Si window layer with a thickness of 0.3µm is staked on top of the a-Si layer to enhance the optical transparency by creating an optical gap. The thickness of the a-Si is varied from 0.5 µm to 1.2 µm and the $J_{sc}$ is optimized.

![Diagram of a single junction a-Si solar cell]

**Figure 5.1** Single Junction a-Si Solar cell

The generation rate is calculated for only 0.5 µm thickness along the x-direction and replicated up to 18 periods to cover the whole geometry of 10.5 µm length in DEVICE. The CAD view of the design, IV curve, power (max), power absorbed, and generation rate are shown in Figure 5.2 and Figure 5.3. Figure 5.2 (b) shows that the optimized short circuit for the design $J_{sc}$ is noticed at 10.959 mA/cm² in DEVICE with an open circuit voltage $V_{oc} = 696.97$ mV. The fill factor and the efficiency are achieved as $FF = 78.985\%$ and $\eta = 6.033\%$ respectively. The $J_{sc}$ for an ideal Si recombination model is around 22 mA/cm², which is around double the $J_{sc}$ noticed as 10.95 mA/cm² in this model. Figure 5.2 (c) shows the $FF = 78.98\%$ and $\eta = 6.03\%$ respectively.
Figure 5.2  

a) CAD view of c-Si/a-Si:H single junction solar cell  
b) Power curve (Efficiency in %)  
c) IV curve
Figure 5.3  

a) Power absorbed at $\lambda = 343$ nm, b) Generation rate at 411 nm, 

c) Total Generation rate exported to DEVICE,  

d) Spectrum response for $\mu$-SiGe  
e) Spectrum response for a-Si
The checkerboard patterns are used for maximum light trapping at the surface of the solar cell. Figure 5.3 (a) shows the profile of optical absorption per unit area at wavelength 343 nm along the y-axis (thickness of layers). It is clear that the absorption increases at the interfaces with the checkerboard patterns. The absorption per unit area (Watt/m²) is normalized to the source power. This absorption portion relative to the incident power is calculated by integrating over the whole area along the thickness (y-axis), shown in Figure 5.3 (a). Absorbed power is proportional to the electric field intensity and the imaginary part of the permittivity. Therefore, the results are given in terms of frequency (or wavelength) domain and permittivity from the index monitor.

The image on the right in Figure 5.3 (b) shows that the absorbed photons (electron and hole pairs) are concentrated at the top surface of each layer and inside the grooves of the checkerboard surface. This generation drops exponentially as it moves into the film along the optimized y-axis. This decrease in optical power is due to the signal degradation inside the silicon layer due to the increase in lifetime, recombination, and impurities. The generation rate is calculated for only 0.50 µm thickness along the x-direction, as is shown in Figure 5.3 (b) and replicated up to 18 periods to cover the entire geometry of 10.50 µm length of the simulated area in DEVICE, as shown in Figure 5.3 (c).

Applying the same model for the µc-SiGe thin film layer as compared to the a-Si thin film improves our results. In amorphous thin film, the S-W (Staebler-Wronski) effect may be weakened by doping Ge atoms and the band gap can be tuned by changing the Ge content. Thus, the spectral response range can be extended to near-infrared by doping an appropriate number of Ge atoms into µc-SiGe thin film (Yan, Zhao, Chen, Wang, Diao, Mao, & Wang, 2013). Since the atomic radius of the Ge atom is larger than the Si atom, the density of defect states would be increased when Ge is doped into the µc-SiGe thin film (Shaoying, Chong, Tao, Jie, & Yu, 2014). We assume that mobility, permittivity, and electron affinity of µc-SiGe thin film are not dependent on Ge content. The spectral response range
is extended to near-infrared by doping the appropriate Ge atoms into $\mu$-SiGe thin film as compared to a-Si thin film, as shown in Figure 5.3 (d) and (e).

The simulation is implemented under the same Schokley-Read-Hall (SRH) recombination and Auger recombination conditions. The trap-assisted lifetime is adjusted for carriers as $1.2 \times 10^{-10}$ s for electron and $0.7 \times 10^{-10}$ s for hole respectively in the SRH recombination. For auger recombination, the capture coefficients for $e = 2.8 \times 31 \text{ cm}^4/\text{s}$ and $h = 9.9 \times 32 \text{ cm}^4/\text{s}$ are adjusted. Considering only the generation rate and totally neglecting any recombination of carriers, the $J_{sc}$ in FDTD is $33.7287 \text{ mA/cm}^2$ and the total generation rate is $1.00492 \times 10^28 (1/\text{m}^2/\text{s}).$ Transporting these values to DEVICE and adjusting the other values to optimize the design, the short circuit for $\mu$-SiGe thin film $J_{sc}$ is $13.3894 \text{ mA/cm}^2$. The increase in the thickness of the layer increases the $J_{sc}$. The IV graph and the Power (max) are shown in Figure 5.4.

Figure 5.4 Power curve (Efficiency in %) and IV curve

The increase in the thickness of the layer increases the $J_{sc}$. The open circuit voltage is $V_{oc} = 626.26 \text{ mV}$. The Fill factor and the efficiency of the device are achieved as $FF = 84.27\%$ and $\eta = 7.06\%$ respectively. The thickness of the $\mu$-SiGe thin film layer varies from $0.50$ to $1.50$ and the optimized values are recorded at $1.20 \mu$m. Figure 5.5 (a) shows the band diagram for the $\mu$-SiGe thin film. The image on the left in Figure 5.5 (b) shows that the generation rate (electron and hole pairs) is
Figure 5.5  a) Band diagram, b) Generation rate at 411nm,

c) Power absorbed at $\lambda = 343$ nm,

d) Total Generation rate exported to DEVICE
concentrated at the top surface of each layer and inside the grove of the checkerboard surface.

Again, the generation rate is calculated for only 0.50 μm thickness along the x-direction and replicated up to 18 periods to cover the entire geometry of a 10.50 μm length of simulated area in DEVICE, which is shown in Figure 5.5 (c). The optical absorption per unit area at wavelength 343 nm along the y-axis (thickness of layers) is shown in Figure 5.5(c). It is clear that the absorption increases at the interfaces with the checkerboard patterns again. The normalized absorption per unit area (Watt/m²) to the source power is shown in Figure 5.5(c).

5.2.2 Double Junction Tandem a-Si/µc-SiGe Solar cell

A two-dimensional numerical simulation of a double junction, thin film tandem solar cell, c-Si/a-Si/µc-SiGe, is designed and investigated to optimize the performance. Both layers are stacked in a way that the a-Si layer is used as the middle absorbing layer and the µc-SiGe layer is the bottom layer. For the design of a double junction solar cell based on the c-Si/a-Si/µc-SiGe design, a very narrow process of parameter space is available for the device optimization due to very tight control of the band gap and low heterojunction quality. To achieve a stable efficiency in an industrial environment, a low defect density is always needed at the interface as well as in the bulk material. The design is shown in Figure 5.6. The use of band-gap engineering is a promising opportunity for optimizing efficiency in a thin film solar cell; however, an S-shaped photocurrent response has been noted in literature due to high band offset between c-Si, a-Si, and a-SiGe, and also because of a very poor-quality interface (Nawaz & Ahmad, 2012). In this study, the band structure is designed considering these challenges and optimizing the efficiency. For a heterojunction tandem design, two junctions are formed at the thickness at 0.3μm between c-Si/a-Si and at 1.5 μm, between a-Si/µc-SiGe along the z direction. The bandgap of the top c-Si window layer is 1.12eV; the middle
a-Si layer is 1.5eV; and the bottom layer 1.7eV. The current and efficiency are optimized by varying the thickness of the main absorbing layers. The simulation is implemented within Lumarical FDTD and DEVICE by considering the Schokley-Read-Hall recombination, Radiative combination, and Auger recombination models. For amorphous Silicon, the radiative recombination model is neglected while it is considered for c-Si with default values of ehp (electron-hole pair) capture rate 1.6e-14 cm²/s. In FDTD, the $J_{sc}$ is noted as 26.227 mA/cm² and the total generation rate is $3.33902e+027$ (1/m²/s). The 2D generation rate is calculated in FDTD with a period of 0.5 µm and repeated along the length up to 10.5 µm (in x direction).

The generation rate in x-y is then flipped over the x-z axis to adjust the 2D simulation into the 3D CAD design DEVICE. Transporting these values to DEVICE and adjusting the interface values between the layers and with Al (used as the metal contact) and Glass ($SiO_2$), the short circuit for the thin film tandem cell $J_{sc}$ is changed to 16.4136 mA/cm².

Figure 5.6 c-Si/a-Si:H/a-SiGe tandem solar cell
Figure 5.7  a) Spectrum response, b) Band diagram, 

c) IV curve, d) Power (max) and efficiency curve.

The voltage applied at the base is varied from 0V to 0.78V while keeping the emitter at 0V. The open circuit voltage is noted as $V_{oc} = 732.323$ mV. The fill factor and the efficiency of the device are $FF = 81.9017\%$ and $\eta = 9.84462\%$ respectively. The IV graph and the Power (max) are shown in Figure 5.7. The increase in the thickness of the layers increases the $J_{sc}$ and reduces the $V_{oc}$. The
thickness of the a-Si and μc-SiGe layers are varied from 0.5 to 1.5 and optimized at 1.2µm and at 1.5µm respectively

5.3 Optimization of design by using different light trapping techniques

There are many ways to enhance photo absorption for wavelengths near IR but the most challenging aspect is to find the best tradeoff between the electrical and optical properties by changing different surface morphologies. The most often used light trapping techniques are the pyramid and moth-eye structure. For silicon wafer-based cells, it is standard to use the pyramid structure, which is several microns in size, to trap light within the solar cell (Campbell & Green, 1987). In this research, we studied and compared different light soaking designs for a thin film solar cell and optimized the efficiency. We compared the efficiencies of pyramidal periodic design, checkerboard periodic design, and quarter pyramid in an empty checkerboard (QPEC) design. The efficiencies of these light trapping techniques are also compared with the light absorbing ability of antireflection coatings (ITO and Si₃N₄). The potential short circuit current density (Jₛₑ) and efficiency of optimized structured is finally compared against the planer cell (cell with an ideal Lambertian scattering). The three different light trapping designs are shown and discussed in the following sections.

5.3.1 Tandem Cell with Pyramidal Design

The 3D design of a tandem solar cell with a pyramid textured design is shown in Figure 5.8. The total thickness of the absorbing layers is 3µm. The dimension of the pyramidal design is 0.5µm by 0.5µm by 0.5µm. The effect of the pyramidal light trapping technique is studied and optimized by varying the height (thickness). Maximum efficacy is recorded at a thickness of 0.5µm. With further increasing the thickness of pyramidal design, the performance of the software was unpredictable due hardware limitations. Overall, the Jₛₑ increases up to 16.957 mA/cm², with a 3.2% increase as compared to the planer solar cell. Vₒc = 737.374 with fill factor FF = 82.071% and efficiency η = 10.262%. The increase in
efficiency is 4.1% as compared to the planer solar cell and 2.17% reduced as compared to ITO and Si$_3$N$_4$.

![Diagram of solar cell with light trapping](image)

**Figure 5.8**  a) Solar cell, b) Focused view of the pyramidal structure, c) IV curve, d) Power (max) and efficiency curve

### 5.3.2 Tandem Cell with Checkerboard Texture Design

The effect of light trapping by the checkerboard technique is studied. Optimum values are calculated. The height (thickness) is varied from 0.25µm to 0.5µm while keeping the x and y dimension constant.
Figure 5.9  a) Solar cell, b) Focused view of the checkerboard design, c) IV curve, d) Power (max) and efficiency curve

The length and width of each square pillar is 0.25µm. Maximum efficacy is recorded at a thickness of 0.5µm. Overall the $J_{sc}$ increases up to 20.2694 mA/cm$^2$, with a 19% increase, as compared to the planer solar cell. $V_{oc} = 742.424$ and fill factor $FF = 82.382\%$. The efficiency of the solar cell increased up to $\eta = 12.397\%$ with the checkerboard trapping technique. The increase in efficiency is 20.5% as compared to the planer solar cell, 17.2% as compared to the pyramidal technique, and 15.42% as compared to ITO and Si$_3$N$_4$. The design is shown in Figure 5.8.

5.3.3 Tandem Cell with Quarter Pyramid in Empty Checker Design (QPEC)

This design is constructed by inserting one-quarter of a pyramid in an empty area of the checkboard. The design is effective in light trapping but it is
more complicated to construct and implement practically in an industrial environment as compared to other light trapping techniques. The design of QPEC is shown in Figure 5.10. The short circuit \( J_{sc} \) increases up to 17.550 mA/cm\(^2\), with a 3.2% increase as compared to the planer solar cell. \( V_{oc} = 738.485 \text{ mV} \) with fill factor \( FF = 82.108 \% \) and \( \eta = 10.8521\% \). The percent increase in efficiency is 9.2% as compared to the planer solar cell and a 3.3% increase as compared to ITO and SI\(_3\)N\(_4\). The efficiency of ITO (TIO\(_2\)) and SI\(_3\)N\(_4\), antireflection coatings is \( \eta = 10.4855\% \). Both ITO and SI\(_3\)N\(_4\) have the same efficiency. The generation rate, \( G \), in FDTD is shown in Figure 5.11. This generation rate is exported from FDTD to DEVICE with a periodic length of 0.5µm as \( G\)-export. The power absorption, \( P_{abs} \), and \( G\)-export are also shown in Figure 5.11 for each of the four designs. Efficiencies of all designs are shown in Table 5.1. Table 5.2 shows the circuit current \( J_{sc} \) and maximum generation rate; this \( J_{sc} \) is recorded in FDTD before considering the recombination processes.

The design is effective in light trapping but it is more complicated to construct and implement practically in an industrial environment as compared to other light trapping techniques. The design of QPEC is shown in Figure 5.10. The short circuit \( J_{sc} \) increases up to 17.550 mA/cm\(^2\), with a 3.2% increase as compared to the planer solar cell. \( V_{oc} = 738.485 \text{ mV} \) with fill factor \( FF = 82.108 \% \) and \( \eta = 10.8521\% \). The percent increase in efficiency is 9.2% as compared to the planer solar cell and a 3.3% increase as compared to ITO and SI\(_3\)N\(_4\). The efficiency of ITO (TIO\(_2\)) and SI\(_3\)N\(_4\), antireflection coatings is \( \eta = 10.4855\% \). Both ITO and SI\(_3\)N\(_4\) have the same efficiency. The generation rate, \( G \), in FDTD is shown in Figure 5.11. This generation rate is exported from FDTD to DEVICE with a periodic length of 0.5µm as \( G\)-export. The power absorption, \( P_{abs} \), and \( G\)-export are also shown in Figure 5.11 for each of the four designs. Efficiencies of all designs are shown in Table 5.1. Table 5.2 shows the circuit current \( J_{sc} \) and the maximum generation rate; this \( J_{sc} \) is recorded in FDTD before considering the recombination processes.
Figure 5.10  a) Solar cell, b) Focused view of QPEC structure, c) IV curve, d) Power (max) and efficiency curve
Figure 5.11 G, G-export, and Pabs for a) Checkerboard, b) pyramidal technique c) QPEC structure d) Planner Solar cell
Table 5.1 Comparing Efficacies between Different Light Capturing Techniques

<table>
<thead>
<tr>
<th></th>
<th>Without texture (planner cell)</th>
<th>Pyramid Design</th>
<th>Checkerboard</th>
<th>Quarter pyramid in empty checker</th>
<th>ITO (TIO₂)</th>
<th>Si₃N₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>J_{sc} (mA/cm²)</td>
<td>16.413</td>
<td>16.957</td>
<td>20.269</td>
<td>17.550</td>
<td>16.813</td>
<td>16.813</td>
</tr>
<tr>
<td>V_{oc} (mV)</td>
<td>732.321</td>
<td>737.374</td>
<td>742.424</td>
<td>738.485</td>
<td>742.424</td>
<td>742.424</td>
</tr>
<tr>
<td>P_{max} (mW/cm²)</td>
<td>9.844</td>
<td>10.262</td>
<td>12.397</td>
<td>10.852</td>
<td>10.485</td>
<td>10.485</td>
</tr>
<tr>
<td>FF (%)</td>
<td>81.901</td>
<td>82.071</td>
<td>82.382</td>
<td>82.108</td>
<td>84.003</td>
<td>84.003</td>
</tr>
</tbody>
</table>

Table 5.2 FDTD Solution Provide the Generation

<table>
<thead>
<tr>
<th></th>
<th>Without texture</th>
<th>Pyramid Design</th>
<th>Checkerboard</th>
<th>Quarter pyramid in empty checker</th>
<th>ITO (TIO₂)</th>
<th>Si₃N₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>J_{sc} (mA/cm²)</td>
<td>26.226</td>
<td>27.587</td>
<td>35.585</td>
<td>33.938</td>
<td>27.534</td>
<td>27.534</td>
</tr>
<tr>
<td>G_{max} (1/cm²/s)</td>
<td>33.390e+27</td>
<td>34.407e+027</td>
<td>90.878e+027</td>
<td>34.278e+027</td>
<td>31.675e+27</td>
<td>31.675e+27</td>
</tr>
</tbody>
</table>

5.4 Buffer layer at the a-Si:H/μc-SiGe Interface

A very thin 1µm intrinsic μc-Si layer is inserted at the a-Si:H/μc-SiGe interface. The efficiency of the tandem cell is increased. The calculations from the study by Keppner, Meier, Torres, Fischer, and Shah (1999) show that the efficiency increases when inserting an a-SiC buffer layer at the interface. However, with the a-SiC, the performance of the device becomes very sensitive to design, band gap,
setting the biased voltage and other parameters, thus functions are easily diverging
with a higher band gap. By inserting the intrinsic μc-Si buffer layer, the response is
unstable at a higher band gap. The initial efficiency of the cell is η = 13.117% at
band gap $E_g = 1.12\text{eV}$ but becomes more stable at $E_g = 0.8 \text{eV}$ with η = 13.06%.
The short circuit $J_{sc} = 21.120 \text{mA/cm}^2$, $V_{oc} = 747.475\text{mV}$, and the fill factor is noted
as FF = 82.76%. The band structure, efficacy diagram, and IV curve are shown in
Figure 5.12.

![Band Diagram](image1)

![IV Curve](image2)

![Power (max) and Efficiency Curve](image3)

**Figure 5.12**  a) band diagram, b) IV curve, c) Power (max) and efficiency curve.

The purpose of inserting this thin layer is to assess the impact of tunneling current
on the efficiency of the device. Due to insertion of this thin layer, the quasi-Fermi
levels come closer to each other and electrons can transfer across the interface; even a small increase potential can start the process of tunneling. The efficiency is increased with insertion of the thin layer because the interface losses are reduced. For higher band gaps with a very thin interface layer, less than 0.05µm, the interface design becomes unstable and an unpredicted current response has been noticed.

5.5 Conclusion

The 2D computer analysis of a tandem solar cell, c-Si/a-Si:H/µc-SiGe, is studied within Lumerical FDTD/Device 4.6. The design is implemented by staking three sub-cells with a band gap of 1.12eV, 1.5eV and 1.7 eV respectively. The optical characterization of the material is performed in FDTD, and then the total generation rate is transported into DEVICE. Electrical characterization is carried out in DEVICE. In the first stage, a single junction solar cell with both a-Si and µc-SiGe absorbing layers are designed and compared. The thickness for both layers are kept the same. In a single junction, a solar cell with an a-Si absorbing layer, the short circuit current is noted as $J_{sc} = 10.959$ mA/cm$^2$, open circuit voltage $V_{oc} = 696.97$ mV, Fill factor $FF = 78.985\%$, and efficacy $\eta = 6.033\%$. Efficiency, short circuit current, and fill factor are increased for µc-SiGe absorbing layer as given $\eta = 7.06671\%$, $J_{sc} = 13.3894$ mA/cm$^2$, and $FF = 84.2753\%$ respectively. The only open circuit voltage reduced for c-Si/µc-SiGe cell is $V_{oc} = 626.263$ mV. In the second stage, implementing the tandem design, with both a-Si as the middle absorbing layer and µc-SiGe as the bottom layer, the efficacy and stability of the device are studied. For the tandem thin film solar cell c-Si/a-Si:H/µc-SiGe, the short circuit $J_{sc} = 16.4136$ mA/cm$^2$, open circuit voltage $V_{oc} = 732.323$ mV, fill factor $FF = 81.9017\%$ and efficiency $\eta = 9.84462\%$.

By applying different light trapping techniques, the device performance is compared. Three different designs are investigated and the efficiencies are compared with the efficiency of a planner solar cell and with anti-light reflecting coatings (TIO$_2$ and SI$_3$N$_4$). The efficiency is optimized with a checkerboard light
trapping design (QPEC), $\eta = 12.397\%$. The increase in efficiency is 20.5% as compared to the planer solar cell, 17.2% as compared to the pyramidal technique, and 15.42% as compared to ITO and $\text{Si}_3\text{N}_4$. In the QPEC technique, the percent increase in efficiency is 9.2% as compared to the planer solar cell and a 3.3% increase as compared to ITO and $\text{Si}_3\text{N}_4$. With the pyramidal design, light trapping increases and efficiency is increased by 4.1% as compared to the planer solar cell and reduced by 2.17% compared to ITO and $\text{Si}_3\text{N}_4$. The efficiencies for both ITO ($\text{TiO}_2$) and $\text{Si}_3\text{N}_4$ antireflection coatings are noted to be the same as $\eta = 10.4855\%$. After stabilizing the parameters, a 0.1$\mu$m thin $\mu$c-Si layer is inserted at the a-Si:H/$\mu$c-SiGe interface to assess the tunneling current. This mechanism further improves the previous interface recombination losses and further improves the efficacy up to $\eta = 13.065\%$. For higher band gap with a very thin interface of less than 0.05$\mu$m, the interface design response becomes unstable and an unpredictable current response has been noticed.
References


Haque, K. E., Quddus, T. N. B., Ferdaous, M. T., & Hoque, M. A. (2013). An analysis of efficiency variation in an Al0.7Ga0.3As/Al0.48In0.52As heterojunction solar cell with change in device parameters using adept 1D software. *Electronic Materials Letters, 9*(1), 47-52.


OFFE Institute online database. Retrieved on July 2015 from:
http://www.ioffe.ru/index_en. html and
http://www.ioffe.ru/SVA/NSM/nk/Germanium
Compounds/Gif/si85ge15.gif


Appendix –A

(Programming script)

To get data from simulation

Gexport = getresult("solar_generation","G_export");
fname = getnamed("solar_generation","export filename");
G1 = Gexport.G;
x1 = Gexport.x;
y1 = Gexport.y;
z1 = Gexport.z;

Flipping axes to match setup in DEVICE

x=x1;
z=y1;
y=z1;
G=permute(G1,[1,3,2]);
image(x,z,pinch(G,2,1));
matlabsave("generation_flip_axes",x,y,z,G);

To plot J-V and V-P curves

dim=get("solver geometry");# 3 is 3D, 0,1,2 are 2D
if(dim<3){
area = getnamed('Device region','norm length')*getnamed("Device region","x span");
}
if(dim==3){
area = getnamed("Device region","x span")*getnamed("Device region","y span");
}
if(area<1e-14){
  "please set correct simulation dimension";
}

area = getNamed('Device region','norm length')*getNamed("Device region","x span");
J_base = pinch( getData("Device region","base.I"))/area;
V_base = pinch(getData("Device region","base.Vs")); # get source voltage
plot(V_base,J_base*0.1,"Voltage [volts]", "Current Density [mA/cm^2]");

area = getNamed('Device region','norm length')*getNamed("Device region","x span");
J_base = pinch( getData("Device region","base.I"))/area;
V_base = pinch(getData("Device region","base.Vs"));
P=-J_base*V_base;
plot(V_base,P*0.1,"Voltage [volts]", "Power [mW/cm^2]");

**To print out values**
Jsc = J_base;
Current=getData("Device region","base.I");
Voltage=getData("Device region","base.V_base");
Voltage_new=linspace(0.5,1,100);
Current_interp= interp(pinch(Current),Voltage, Voltage_new);
Voc = Voltage_new(find(Current_interp,0));
"Jsc(min) = " + num2str(min(Jsc)*0.1) + " mA/cm2"
"Voc = " + num2str(Voc*1000) + " mV"
"p(max) = " + num2str(max(P*0.1)) + " mW/cm^2";
?"FF = " + num2str((max(P)/(Voc*min(Jsc)*0.01))) + "%";
?"eta = " + num2str(max(P*0.1)) + "%";

#? getdata("Device region","emitter.I")/(getnamed('Device region','norm length')*getnamed("Device region","x span"));
#? getdata("Device region","base.I")/(getnamed('Device region','norm length')*getnamed("Device region","x span"));

#########################################################################
# Scriptfile: solar_cell_incoherent.lsf
# This script creates a file containing the generation profile using an incoherent source
# Copyright 2012, Lumerical Solutions, Inc (Solutions, F. D. T. D., 2016).
#########################################################################
# Run two simulation; one for each source.
# incoherent interference can be obtained

# run simulation with source 1
switchtolayout;
setnamed("s1","polarization angle",0);
save("temp1");
run;
runanalysis;

Jsc_1=getdata("solar_generation","Jsc");
G_1=getresult("solar_generation","G_export");
# run simulation with source 2
switchtolayout;
setnamed("s1","polarization angle",90);
save("temp2");
run;
runanalysis;

Jsc_2=getdata("solar_generation","Jsc");
G_2=getresult("solar_generation","G_export");

#Coherently average the results of the two polarization simulations
Jsc=0.5*(Jsc_1+Jsc_2);
Ga=0.5*(G_1.G+G_2.G);

#Print the results of the incoherent simulation
"Normalized short circuit current is : " +num2str(Jsc) + " A/m^2";
"Maximum generation is : " + num2str(max(Ga))+ " 1/m^3/s";

#Plot results and export
x=G_2.x;
y=G_2.y;

image(x*1e6,y*1e6,log10(pinch(G_1.G,3,1)),"x (um)","y (um)", "Generation (Log scale) - pol=0");
image(x*1e6,y*1e6,log10(pinch(G_2.G,3,1)),"x (um)","y (um)", "Generation (Log scale) - pol=90");
image(x*1e6,y*1e6,log10(pinch(Ga,3,1)),"x (um)","y (um)", "Generation (Log scale)- Unpolarized");
#Export to DEVICE

# rotate axes

x=G_2.x;

y=G_2.z;

z=G_2.y;

G = permute(Ga,[1,3,2]);

matlabsave("generation_rectangular_incoherent",x,y,z,G);

########################################################################

# Export to DEVICE

# rotate axes

x=G_2.x;

y=G_2.z;

z=G_2.y;

G = permute(Ga,[1,3,2]);

matlabsave("generation_rectangular_incoherent",x,y,z,G);

########################################################################