CHAPTER – 4
Simulation assisted Design of Single Junction Hydrogenated Amorphous Silicon Thin Film Solar Cells

A single junction a-Si:H TFSC is investigated with the use of single dimensional numerical simulation tool for understanding the role of device parameters and its variations on the device absorption. The device model is developed to understand the correlation between the incident photons to e-h pair generation to the generated current. With the basic understanding of the material properties of a-Si:H and constituent developed p-i-n model, computational design and analysis are performed to understand a-Si:H as a TFSC material. This chapter covers details of the device modelling, structural description and the simulation results covering all the possible device patterns.

4.1. Modelling of Device Structure

The cost-effective way of designing the system is to perform the analytical simulation to understand the behavioural pattern before proceeding with the fabrication. Hence for our problem statement to derive an efficient single junction a-Si:H TFSC, an optimal model is developed covering all aspects from incident light to absorption to e-h pair generation to device current to output power. The defined model is described in chapter systemically covering Poisson’s transport equation and details of single dimensional AFORS-HET simulation software for solving the equations.

4.1.1. Poisson’s transport Equation

The developed model should be able to electrically simulate the structure, using the fundamental semiconductor physics at all nodes of the mesh by solving Poisson’s equations, charge transport of drift-diffusion equations and carrier continuity equations for holes and electrons [149]. Under the influence of incident radiations, an electrostatic potential change to charge density within the semiconductor device is explored by Poisson equation. The transport equations and the charge carrier continuity equations describe the hole and electron densities as a result of transport, generation and recombination process.
Poisson equation: \[ \nabla^2 \phi = \frac{\rho}{\varepsilon_0 \varepsilon_r} = \frac{q (p + N_D - n - N_A)}{\varepsilon_0 \varepsilon_r} \quad (4.1) \]

Equations for charge carrier continuity:
\[
\begin{align*}
\frac{\partial n}{\partial t} &= \frac{1}{q} \nabla \cdot J_n + G_n - R_n \\
\frac{\partial p}{\partial t} &= \frac{1}{q} \nabla \cdot J_p + G_p - R_p 
\end{align*} \quad (4.2) \]

Charge transport equations:
\[
\begin{align*}
J_n &= qn \mu_n \varepsilon + qD_n \nabla n \\
J_p &= qp \mu_p \varepsilon + qD_p \nabla p 
\end{align*} \quad (4.4) \]

\[
\begin{align*}
J_n &= qn \mu_n \varepsilon + qD_n \nabla n \\
J_p &= qp \mu_p \varepsilon + qD_p \nabla p 
\end{align*} \quad (4.5) \]

where, \( \phi \) is the electrostatic potential, \( \rho \) the total charge density, \( q \) the electric charge, \( \varepsilon_0 \) the permittivity of free space, \( \varepsilon_r \) the relative permittivity of semiconductor, \( n \) and \( p \) are number of charge carriers, \( N_A \) and \( N_D \) are acceptor and donor impurity concentrations, \( G_p \) and \( G_n \) are the hole and electron generation rates, \( \mu_p \) and \( \mu_n \) are the hole and electron mobility, \( R_p \) and \( R_n \) are the hole and electron recombination rates, \( J_p \) and \( J_n \) are the hole and electron current density and \( \varepsilon \) is the electric field.

The electronic properties of optoelectronic devices are basically defined by the transport properties determined by drift and diffusion currents, which are the two basic conduction mechanisms in the semiconductor. Drift Current (\( I_d \)) is the motion of charged carriers under the electric field influence, flowing in the direction similar to that of applied field or applied voltage. Contrary to that, Diffusion Current (\( I_{Diff} \)) is the motion of charges due to the concentration gradient change. The sum of diffusion and drift current density of holes and electrons describes the total current density (\( J_{total} \)).

Drift Current: \[ I_d = \mu \cdot \varepsilon \cdot q \cdot n \cdot A \quad (4.6) \]

Diffusion Current: \[ I_{Diff} = q \cdot D \cdot A \cdot \frac{dn}{dx} \quad (4.7) \]

Total Current density: \[ J_{total} = q \cdot \varepsilon (n \cdot \mu_n + p \cdot \mu_p) + q \left( Dn \frac{dn}{dx} - Dp \frac{dp}{dx} \right) \quad (4.8) \]
where $\mu_p$ and $\mu_n$ are the mobilities of hole and electron, $p$ and $n$ are the hole and electron carrier density, $D_p$ and $D_n$ are the hole and electron diffusion coefficient and $E$ is the applied electric field in the $x$ direction.

### 4.1.2. Description of Single-Dimensional AFORS-HET Software

The single dimensional AFORS-HET software solves the semiconductor equations consisting of Poisson equation, electrons and holes continuity and transport equation under multiple diverse modes of operation with the help of finite differences [150]. The e-h pair generation can be defined by plain surface calculation for coherent/incoherent internal multiple reflections by using the complex reflection indices for the layers or Lambert-Beer absorption covering the rough surfaces by using measured transmission and reflection files. All the internal device quantities like Fermi energies, band diagrams, phase shifts, cell currents and local recombination/generation rates can be calculated. The added advantage of this program is it provides multidimensional parameter fitting and arbitrary parameter variations in order to obtain a clear matching between simulated measurements to real measurements. The basic input parameter for the simulation models constitutes of incoming spectral photons with the semiconductor layer dielectric properties defined by the complex refractive index: $N(\lambda) = n(\lambda) + i k(\lambda)$, here $k(\lambda)$ and $n(\lambda)$ denote extinction coefficient and refractive index respectively. All the semiconductor layers are defined by dimensional parameters like thickness, electron/hole mobilities, band densities, thermal velocities, doping profiles as mentioned in Table 4.1. The generation of device current depends on the electron-hole pair generation and recombination, a radiative recombination model is incorporated into defining property to account for the realistic simulations. The semiconductor layer interface are assumed to be ohmic for the ease of design and reducing the run time, picking the “drift-diffusion interface” model for covering both drift and diffusion currents across the interfaces. The developed solar cell can be characterized in terms of current-voltage (IV) plots.

### 4.2. Structural Description of Single Junction a-Si:H TFSC

The high dangling bond density in a $n$-or $p$-type doped a-Si:H leads to light-induced charge carriers loss in $p$-$n$ junction due to recombination. Hence, an intrinsic material is introduced between $p$-and $n$-type where the majority of the charge carriers are generated and drifts to the external contacts due to the internal electric field influence [151]. The a-Si:H TFSC can be either
n-i-p or p-i-n structures based on the sequence of doped and intrinsic layer depositions. The considered p-i-n approach, termed as superstrate configuration is the most preferred option making the light to enter the device through p-layer, as the mobility of holes is lower compared to the mobility of electrons for thin film layers. The sequence of p, i, n deposition is grown on TCO coated glass substrates for concentrating the incident radiations into the device as they exhibit higher optical transmission. The p-layer behaves as the window for the electrical layers in the device to i-layer which absorbs the light further generating e-h pairs and due to its built-in potential, junction field separates holes and electrons and they travel to p-layer and n-layer respectively resulting in flow of photocurrent within the cell. The electrons and holes generated in p-and n-type layers do not contribute to the device current due to their shorter lifetime. But p and n-type layers create an electric field in the undoped intrinsic absorber layer in order to collect the photo-generated e-h pairs completing the circuitry. The short carrier diffusion lengths of direct bandgap a-Si:H requires thickness in nanometer range for the current generation. For the thin film device functionality, the p-layer and n-layer’s are restricted to few nanometers ranging anywhere between 10-30nm to generate an electric field throughout the intrinsic i-layer of around 300-500nm. Fig. 4.1(a) shows the superstrate single junction p-i-n structured a-Si:H TFSC.

![Figure 4.1. Designed p-i-n configuration of a-Si:H PV device](image)

For the device structure, optical enhancement is achieved by the highly absorbing incident light from transparent conducting oxides (TCO) at front surface and by effectively reflecting light back into the cell from the rear metal layer. P-type doped TCO’s such as Indium Tin Oxide (ITO) and Zinc Oxide (ZnO) deposited on the glass serves as the wideband window in collecting photo-
current by providing transparency for solar illumination. The rear metallic layer with an ohmic contact with \( n \)-layer helps in reflecting long wavelength light which is poorly absorbed in a-Si:H in turn suppressing the range of radiations going out of the device. In addition to the device structure, quality of the materials also play a very key role for efficiency enhancement.

**4.3. Performance Parameters of Photovoltaic Device**

The PV device functionality is validated generally by following output parameters: short circuit current density (\( J_{sc} \)), open-circuit voltage (\( V_{oc} \)), Fill Factor (\( FF \)) and efficiency (\( \eta \)). The junction built-in voltage (\( V_{bi} \)) across the undoped i-layer is dependent on the doping concentration given by

\[
V_{bi} = \frac{kT}{q} \ln \left( \frac{N_A \cdot N_D}{N_i^2} \right) \tag{4.9}
\]

where, \( T \) is the temperature, \( q \) denotes the electronic charge, \( k \) the Boltzmann’s constant, \( N_A \) and \( N_D \) are \( p \)-and \( n \)-type layer doping concentrations respectively.

**Figure 4.2.** Typical J-V characteristics of a photovoltaic device

The Current density-voltage (J-V) output characteristics of a typical photovoltaic device under the light illumination are as shown in Fig.4.2. The photogenerated current of solar cell is device area dependent, hence current density (\( J \)) is standard considered for calculation of cell efficiency. The device operation at zero bias voltage gives \( J_{sc} \) and an open circuit operation gives \( V_{oc} \) across
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the terminals. The $V_{bi}$ due to the generated e-h pairs across the junction outside the ambit of recombination gives $V_{oc}$ written in a simplified form as

$$V_{oc} = V_{bi} - \text{Recombination Influence} \quad (4.10)$$

$J_{sc}$ is directly dependent on the absorbed solar power and rate of excited electrons by the solar cell, so it completely depends on the optical properties of the PV device. It can be directly obtained by integrating the photogenerated charges under solar irradiance given by

$$J_{sc} = \frac{e}{hC} \int \lambda n_A(\lambda) S(\lambda) d\lambda \quad (4.11)$$

Where $A$ is the semiconductor area, $S(\lambda)$ is the solar irradiance spectrum, $\eta_A(\lambda)$ is the absorption spectrum and $e$ the elementary charge.

The maximum power point determines the $FF$ of the solar cell, limiting the separation and extraction of the photogenerated device charges and is given by

$$FF = \frac{V_m * J_m}{V_{oc} * J_{sc}} = \frac{P_m}{V_{oc} * J_{sc}} \quad (4.12)$$

The ratio of maximum generated electrical power to incident solar power gives the power conversion efficiency, written in simplified form as

$$\frac{P_m}{P_{in}} = \frac{FF * V_{oc} * J_{sc}}{P_{in}} \quad (4.13)$$

where $V_m$ and $J_m$ denote maximum voltage and current density across the device. The incident power and maximum generated power upon light incidence are denoted by $P_{in}$ and $P_m$. The dependence of $\eta$ on $V_{oc}$, $J_{sc}$ and $FF$ are established in above equations as presented in Fig.4.2 and all the three parameters need to be optimized for $\eta$ enhancement in thin film solar cell.

4.4. Simulation Results

A novel single junction a-Si:H TFSC is investigated for understanding the influence of various parameters such as layer thickness, $p$- and $n$-type doping concentrations, bandgap, TCOs as textured and plane surfaces with graded structures on $\eta$ of the device. The trade-off between input parameters were examined in terms of $J_{sc}$, $V_{oc}$, $FF$ and $\eta$ as a function of different structural
variations. The front to back layer systematic approach of investigation is done and the output parameters are tabulated with varied layer configurations to get a clear understanding on the relative improvements over the input parameter variations and helps in optimizing the parameters for solar cell design.

![Figure 4.3. Gaussian Defect density distribution considered for simulations in the doped and undoped a-Si:H layers](image)

The spectrum radiation of AM1.5 with 100mW/cm² incident power density is used as an illuminating source for the carried out device simulations. The Gaussian varying defects as shown in Fig.4.3 were considered for the electrical $p$, $i$, $n$ layers. $E_c$ and $E_v$ are conduction and valence band energy levels respectively, blue and red curve denotes donor and acceptor dangling bonds respectively within the layers. The material properties taken from Zhao et al [152] are used for the simulation based on their doping regions as mentioned in Table 4.1. The optical parameters constituting of refractive index $n$ and reflectivity $k$ for all the constituent layers are obtained from SOPRA Database [153].

The structured way of analysis is performed through simulations by varying the thickness, bandgap and doping concentrations from front $p$ to $n$ layer with the optimized optical layers in front and back TCO inclusive of backscattering metal. Basic structure constituting of $p$, $i$, $n$ layers with the thickness of 10nm, 500nm, 30nm respectively, bandgap of 1.74eV for all electrical layers with a doping concentration of $10^{18}$cm⁻³ for acceptor P-layer and $10^{20}$cm⁻³ for donor N layer is simulated. The obtained output parameter values of $V_{oc}$, $J_{sc}$ and $FF$ are 741mV, 11.92mA/cm² and 0.64 respectively for simulated structure obtaining an efficiency of 5.65% across the device. Further input parameter changes are done to the structures to analyze the scale of variations and comparative efficiency enhancements are analyzed to obtain high energy efficient combination of
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Naming conventions are followed for the samples to determine the type variants: sample numbers with the suffix ‘A’ are for optical layer variants, ‘B’ for p-layer variants, ‘C’ for i-layer variants, ‘D’ for n-layer variants and ‘E’ for graded structures.

**Table 4.1.** Parameters of doped (p/n-type) and undoped a-Si:H layers considered for simulation [152]

<table>
<thead>
<tr>
<th>Parameters</th>
<th>P-type doped a-Si:H layer</th>
<th>Undoped Intrinsic a-Si:H layer</th>
<th>N-type doped a-Si:H layer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bandgap(eV)</td>
<td>Variable</td>
<td>Variable</td>
<td>Variable</td>
</tr>
<tr>
<td>Electron affinity(eV)</td>
<td>3.9</td>
<td>3.9</td>
<td>3.9</td>
</tr>
<tr>
<td>Dielectric constant</td>
<td>11.9</td>
<td>11.9</td>
<td>11.9</td>
</tr>
<tr>
<td>Tauc plot based optical bandgap (eV)</td>
<td>1.74</td>
<td>1.72</td>
<td>1.74</td>
</tr>
<tr>
<td>Hole mobility in a-Si:H (cm²V⁻¹s⁻¹)</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Electron mobility in a-Si:H (cm²V⁻¹s⁻¹)</td>
<td>5</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Thickness of thin film layers (nm)</td>
<td>Variable</td>
<td>Variable</td>
<td>Variable</td>
</tr>
<tr>
<td>Eff. valence band carrier density(cm⁻³)</td>
<td>1x10²⁰</td>
<td>1x10²⁰</td>
<td>1x10²⁰</td>
</tr>
<tr>
<td>Eff. conduction band carrier density(cm⁻³)</td>
<td>1x10²⁰</td>
<td>1x10²⁰</td>
<td>1x10²⁰</td>
</tr>
<tr>
<td>Hole (Auger recombination coeff.) (cm⁶s⁻¹)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Electron (Auger recombination coeff.) cm⁶s⁻¹)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Hole Thermal velocity(cm.s⁻¹)</td>
<td>1x10⁷</td>
<td>1x10⁷</td>
<td>1x10⁷</td>
</tr>
<tr>
<td>Electron Thermal velocity (cm.s⁻¹)</td>
<td>1x10⁷</td>
<td>1x10⁷</td>
<td>1x10⁷</td>
</tr>
<tr>
<td>Acceptor (Doping concentration) (cm⁻³)</td>
<td>Variable</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Donors (Doping concentration) (cm⁻³)</td>
<td>0</td>
<td>0</td>
<td>Variable</td>
</tr>
<tr>
<td>Recombination coeff. (band to band) (cm³s⁻¹)</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Thin film material density(g.cm⁻³)</td>
<td>2.328</td>
<td>2.328</td>
<td>2.328</td>
</tr>
</tbody>
</table>

4.4.1.  **Front and Rear Optical layer variations**

The structures with low conductive amorphous layers having the thickness in nanometer range need highly conductive transparent layers to have carriers into the device. ITO and ZnO are the two generally considered TCO layers and are considered for simulation. The p doped TCO’s thickness is varied from 100 to 1000nm and the obtained output parameters show continuous improvement from 100 to 400nm, further increase didn’t have any positive impact on the absorption. So, with the thickness of 400nm simulative analysis is done. Silver as back metal contact is taken as reference and thickness is varied from 100 to 1000nm, optimized $J_{sc}$ is obtained with 100nm thickness and remains constant for further increase in thickness. As a result, $\eta$ is unaltered with an increase in thickness making it independent of rear metal thickness. Further, the TCO layer has been induced between N-layer and back metal to increase short circuit by reducing...
optical losses at back contact. Optical layers added to structures to analyze their influence on the TFSC operation and the output parameters tabulated in Table 4.2 shows that $J_{sc}$ is drastically enhanced with constant $V_{oc}$ and $FF$, as a result efficiency improvements are on scale to that of $J_{sc}$ enhancement. ITO is better compared to ZnO as TCO optical layer based on sample no.A2 and A4 results with an added practical advantage of excellent anti-reflection coating. It is observed by the obtained results that the optimized TCO films and TCO/metal back reflectors help in minimizing the reflection losses, thermodynamic efficiency, charge carrier separation efficiency and charge collection efficiency providing an efficient light trapping option.

<table>
<thead>
<tr>
<th>Structure</th>
<th>$V_{oc}$ (mV)</th>
<th>$J_{sc}$ (mA/cm$^2$)</th>
<th>FF</th>
<th>$\eta$ (%)</th>
<th>Sample no</th>
</tr>
</thead>
<tbody>
<tr>
<td>ITO(400nm)/P(10nm)/I(500nm)/N(30nm)</td>
<td>747.45</td>
<td>15.6</td>
<td>0.63</td>
<td>7.34</td>
<td>A1</td>
</tr>
<tr>
<td>ITO(400nm)/P(10nm)/I(500nm)/N(30nm)/Silver(100nm)</td>
<td>747.45</td>
<td>15.72</td>
<td>0.63</td>
<td>7.40</td>
<td>A2</td>
</tr>
<tr>
<td>ITO(400nm)/P(10nm)/I(500nm)/N(30nm)/ITO(50nm)/Silver(100nm)</td>
<td>747.45</td>
<td>15.84</td>
<td>0.63</td>
<td>7.45</td>
<td>A3</td>
</tr>
<tr>
<td>ZnO(400nm)/P(10nm)/I(500nm)/N(30nm)/Silver(100nm)</td>
<td>747.42</td>
<td>15.03</td>
<td>0.59</td>
<td>6.6</td>
<td>A4</td>
</tr>
</tbody>
</table>

### 4.4.2. $P$-layer variations

The radiations incident onto the device pass-through TCO to enter $p$-layer, range of absorption and e-h recombination are decided by the material bandgap and the concentration respectively. The performed parameter variations can have material property as input parameter varied to monitor output parameters. Sample no.A2 is considered for varying $p$-layer bandgap from 1.7 to 2.3eV with bandgaps of $i$ and $n$ layers set to 1.72eV and 1.7eV respectively to illustrate the role of $p$-layer bandgap on the device absorption. The output parameter variations for the varying bandgap are as presented in Fig.4.4. There is a continuous increase observed in $V_{oc}$ with bandgap increase from 1.7 to 2eV as the photon absorption is increased at $i$-layer generating more e-h pair and saturates with increasing bandgap range [154]. Majority of the generated e-h pair recombines before separating and heat loss due to the excess photon absorption results in almost constant $J_{sc}$ over the bandgap range. $FF$ is constantly enhanced till 2.2eV and starts decreasing with further increase in the bandgap, the maximum $\eta$ increases from 1.8 till 2.2eV and reduces further following the $FF$. Maximum $\eta$ is observed with a wide band gap of 2.2eV, hence finalized for further
calculations. The low resistive $p$-layer exhibits high conductivity with wider bandgap reduces the absorption related losses [155] in-turn obtaining higher $V_{oc}$. The $p$-layer thickness is considered as 10nm based on reported literature [156, 157] and discussion with companies engaged in practical products. This 10nm is considered as optimum thickness based on factors including, carrier trapping, enhanced hole transport towards $p$-layer contact, maximum light transfer to the carrier generation region namely i-layer and ease of fabrication. The output parameters for varying $p$-layer bandgap and doping concentration are tabulated in table 4.3.

Figure 4.4. Influence of the optical bandgap of $p$, $i$, $n$ layers on the $V_{oc}$, $J_{sc}$, $FF$ and $\eta$ on the a-Si:H PV device

Sample no.B2 with bandgap of 2.2 eV and acceptor concentration of $1 \times 10^{18}$ cm$^{-3}$ shows up the maximum $\eta$. Sample no.B2 is with ITO and sample no.B5 with ZnO, with improvements compared to sample no.A2 and sample no.A4 respectively in table 4.3. Increase in concentration leads to heat losses and decrease in concentration leads to higher recombination, optimized doping concentration is obtained to have higher $FF$ to enhance efficiency [158].
Table 4.3. Influence of tailoring of P-layer bandgap and doping concentration on efficiency of p-i-n configuration

<table>
<thead>
<tr>
<th>Structure</th>
<th>Voc (mV)</th>
<th>J_sc (mA/cm²)</th>
<th>FF</th>
<th>η (%)</th>
<th>Sample No</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample no A2 (E_g=2.2eV and Na=1x10^{16} cm^{-3})</td>
<td>729.63</td>
<td>13.68</td>
<td>0.7</td>
<td>6.98</td>
<td>B1</td>
</tr>
<tr>
<td>Sample no A2 (E_g=2.2eV and Na=1x10^{18} cm^{-3})</td>
<td>729.63</td>
<td>13.73</td>
<td>0.75</td>
<td>7.51</td>
<td>B2</td>
</tr>
<tr>
<td>Sample no A2 (E_g=2.2eV and Na=1x10^{20} cm^{-3})</td>
<td>711.72</td>
<td>12.94</td>
<td>0.79</td>
<td>7.27</td>
<td>B3</td>
</tr>
<tr>
<td>Sample no A2 (E_g=2.2eV and Na=1x10^{22} cm^{-3})</td>
<td>670.97</td>
<td>12.42</td>
<td>0.82</td>
<td>6.83</td>
<td>B4</td>
</tr>
<tr>
<td>Sample no A4 (E_g=2.2eV and Na=1x10^{18} cm^{-3})</td>
<td>727.01</td>
<td>13.04</td>
<td>0.75</td>
<td>7.11</td>
<td>B5</td>
</tr>
</tbody>
</table>

4.4.3. I-layer variations

In this section, bandgap and thickness of i-region are varied keeping other layer parameters constant. Fig.4.4 depicts V_oc, J_sc, FF and η variation for varying i-layer bandgap from 1.7 to 2.2eV, where p and n layer bandgap is set at 2.2 and 1.74eV respectively. Since p-layer bandgap is set to 2.2eV, light with energy less than that will only reach intrinsic layer and so bandgap variations are considered till 2.2eV. The number of photons absorbed are more leading to absorption losses in form of heat at lower i-layer bandgap, resulting in lower η and upon increasing the bandgap from 1.8 to 1.9eV, enhancement in V_oc is observed due to decreased recombination current with proper quasi-fermi level splitting as holes and electrons move to respective layers and decrease in J_sc is seen due to absorption losses attaining lowest at 1.9eV. FF being inversely proportional to J_sc attains maximum value at 1.9eV and due to higher e-h pair generation compared to losses; maximum η follows FF to attain maximum value at 1.9eV. So, for further investigation bandgap of i-layer is set to 1.9eV. Sample no.C1 and sample no.C2 variations in below mentioned Table 4.4 are with respect to sample no.B2 and sample no.B5 respectively. The thickness of undoped i-layer is effectively set to 500nm, a decrease in thickness reduces J_sc further reducing the η as in sample no.C3, enhancement in the i-layer thickness will increase the light absorption but will also increase the probability of e-h recombination and hence decreases the photo-current and the V_oc. Table 4.4 summarizes that with an increase in bandgap, η is improved and in turn reduced by reducing thickness.
Table 4.4. Influence of Intrinsic layer and N-type doped layer thickness on the solar cell efficiency

<table>
<thead>
<tr>
<th>Structure</th>
<th>Voc (mV)</th>
<th>Jsc (mA/cm²)</th>
<th>FF</th>
<th>η (%)</th>
<th>Sample No</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample no. B2 (Eg=1.9eV)</td>
<td>830.25</td>
<td>13.02</td>
<td>0.87</td>
<td>9.40</td>
<td>C1</td>
</tr>
<tr>
<td>Sample no. B5 (Eg=1.9eV)</td>
<td>828.66</td>
<td>12.43</td>
<td>0.82</td>
<td>8.44</td>
<td>C2</td>
</tr>
<tr>
<td>ITO(400nm)/P(10nm)/I(250nm)/N(30nm)/ITO(50nm)/Silver(100nm)</td>
<td>788.66</td>
<td>9.98</td>
<td>0.65</td>
<td>5.12</td>
<td>C3</td>
</tr>
<tr>
<td>ITO(400nm)/P(10nm)/I(500nm)/N(20nm)/ITO(50nm)/Silver(100nm)</td>
<td>746.11</td>
<td>12.95</td>
<td>0.87</td>
<td>8.40</td>
<td>D1</td>
</tr>
<tr>
<td>ITO(400nm)/P(10nm)/I(500nm)/N(32nm)/ITO(50nm)/Silver(100nm)</td>
<td>833.16</td>
<td>13.11</td>
<td>0.85</td>
<td>9.29</td>
<td>D2</td>
</tr>
</tbody>
</table>

4.4.4. N-layer variations

The bandgap, thickness and doping concentration variations of n-type doped layer are considered in this section with p and i layer bandgaps set to 2.2 and 1.9eV respectively. The n-layer absorbs incident light of energy levels between 1.74 to 1.9eV as a result variations are checked only in this bandgap range. Fig.4.4. shows $V_{oc}$, $J_{sc}$, FF and $\eta$ variations with respect to n-bandgap variations. $V_{oc}$ and $J_{sc}$ almost remain constant as n-layer just gets the electrons generated from the undoped i-layer. Light radiations of higher bandgap are reflected back to i-layer for generating e-h pairs [159]. The $\eta$ values show an oscillatory behaviour from 1.7 to 1.74 eV as it’s on rise and dips from 1.75 to 1.85eV and starts increasing again. So bandgap of 1.74eV is best to obtain the maximum $\eta$ and hence considered for the calculations. No changes are observed in $V_{oc}$, $J_{sc}$, FF and $\eta$ with n-layer concentration change from $10^{18}$ to $10^{22}$ cm$^{-3}$. Irrespective of the doping concentration, n-layer just collects the generated electrons with thickness playing a key role in grasping electrons. At a thickness of 30nm maximum $\eta$ is obtained. With further increase in thickness of n-layer, FF will be reduced as electrons have to travel longer distance towards holes and in case of a decrease in thickness, the potential difference across the junctions will drop due to an insufficient thickness to grasp holes. It’s observed that output parameters of the simulated structure with the thickness of 20 and 32 nm are less compared to sample no. C1 as shown in Table 4.4.

4.4.5. Graded Structures (Variation within layers)

Structures constituting of varying concentration and bandgap within layers are considered to understand the impact on output parameters and are relatively compared to constant parameter...
layered structures. Graded structures of this kind are tried out by varying parameters of sample no.C1 and constituent output parameters are tabulated in Table 4.5. With bandgap variation within $p$-layer, $V_{oc}$ is increased due to higher e-h generation whereas higher recombination current leads to a decrease in $J_{sc}$ with higher bandgaps.

Table 4.5. Structures with concentration and bandgap grading of $p$, $i$, $n$ layers

<table>
<thead>
<tr>
<th>Structure</th>
<th>$V_{oc}$ (mV)</th>
<th>$J_{sc}$ (mA/cm$^2$)</th>
<th>FF</th>
<th>$\eta$ (%)</th>
<th>Sample No</th>
</tr>
</thead>
<tbody>
<tr>
<td>P-layer bandgap variation from TCO to I-layer: Sample no.C1 with decrease</td>
<td>737.86</td>
<td>7.47</td>
<td>0.58</td>
<td>3.19</td>
<td>E1</td>
</tr>
<tr>
<td>from 2.1 to 1.74eV</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-layer bandgap variation from TCO to I-layer: Sample no.C1 with increase</td>
<td>830.5</td>
<td>11.07</td>
<td>0.66</td>
<td>6.06</td>
<td>E2</td>
</tr>
<tr>
<td>from 1.74 to 2.1eV</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>P-layer concentration variation from TCO to I-layer: Sample no.C1 with increase from $10^{18}$ to $10^{20}$ cm$^3$</td>
<td>767.42</td>
<td>19.91</td>
<td>0.84</td>
<td>12.83</td>
<td>E3</td>
</tr>
<tr>
<td>P-layer concentration variation from TCO to I-layer: Sample no.C1 with increase from $10^{16}$ to $10^{18}$ cm$^3$</td>
<td>984.9</td>
<td>15.88</td>
<td>0.75</td>
<td>11.73</td>
<td>E4</td>
</tr>
<tr>
<td>I-layer bandgap variation from P-layer to N-layer: Sample no.C1 with decrease from 2.1 to 1.9 eV</td>
<td>863.35</td>
<td>20.13</td>
<td>0.75</td>
<td>13.03</td>
<td>E5</td>
</tr>
<tr>
<td>I-layer bandgap variation from P-layer to N-layer: Sample no.E2 with decrease from 2.1 to 1.9 eV</td>
<td>861.38</td>
<td>19.64</td>
<td>0.75</td>
<td>12.68</td>
<td>E6</td>
</tr>
<tr>
<td>N-layer bandgap variation from I-layer to back TCO: Sample no.E4 with decrease from 1.9 to 1.74 eV</td>
<td>863.35</td>
<td>20.07</td>
<td>0.75</td>
<td>12.99</td>
<td>E7</td>
</tr>
</tbody>
</table>

The simulated results of sample no.E1 and sample no.E2 mentioned in table 4.5 shows us that $FF$ and $\eta$ are influenced by higher recombination current resulting in lower value compared to sample no.C1. Concentration variation within $p$-layer gives higher chance of e-h pair generation and reducing recombination current with lower heat losses resulting in higher $V_{oc}$ and $J_{sc}$, in-turn $\eta$ is enhanced as illustrated in sample no.E3 and sample no.E4. With $p$-layer bandgap set to 2.1eV and variations are done in $i$-layer to understand the impact on the output parameters. Compared to $i$-layer structure with constant bandgap at 1.9eV, if its varied from 2.1 to 1.9eV higher range of light radiations are absorbed to generate higher e-h pairs and with reduced recombination current leading to higher $V_{oc}$, $J_{sc}$ and maximum $\eta$. Sample no.E5 results show an enhanced $\eta$ of graded
structures compared to constant bandgap. On bandgap narrowing of n-layer from 1.9 to 1.74 eV, sample no. E7 shows slightly $\eta$ than sample no. E4. Table 4.5 data indicate that fine tuning of the bandgap within the p, i & n layers in the structure leads to better $V_{oc}$, $J_{sc}$ and $\eta$. In the range of data studied the enhancement in scattering and optical path length of the Incident light greater enhance $J_{sc}$, but do not have significant influence on $V_{oc}$ and $FF$ as the potential at the junctions is unaltered. However, TCO and metal back contact layer stack needs to be optimized for higher stabilized efficiency by introducing higher reflectivity of the incident radiations, minimize loss through passing out of the device [160]. Silver in sample no. C1 when replaced by Aluminum resulted in $J_{sc}$ of 12.90 mA/cm$^2$ with $\eta$ of 9.52%. It is evident that ITO/silver contacts are far superior compared to other noble metals as highest $J_{sc}$ is obtained with Silver but for large area depositions Aluminum can also be preferred purely on cost-effectiveness.

**Summary:** Discussed in this chapter is a comprehensive simulation based study of the role of various parameters including $p$, $i$, and $n$ layer bandgaps, thickness, surface of TCO, and the doping concentration of layers on the conversion efficiency of the a-Si:H TFSC. The analysis is done using a single dimensional software, following the light radiation path from the point of incidence on the surface to absorption to back reflection. The study results show that $V_{oc}$ is influenced by doping concentration and bandgap of layers, $J_{sc}$ by improving the optical path length, leading to higher $\eta$. In the range of data simulated, a simple p-i-n structure showed maximum efficiency of 9.40% (sample no. C1). When the structure was modulated by fine-tuning the bandgap, concentration and thickness of electrical layers efficiency of up to 13.03% (sample no. E5) were obtained during simulation. The simulative design enabled us to understand the material and device properties and to verify the feasibility for growing materials with nearby properties for growth of solar cells. Thus helping to accelerate the feasibility study. Hence based on this data, in a short time the growth and characterization of the $p$, $i$, and $n$ type layers and the device fabrication were carried out in the indigenously developed cluster PECVD system and demonstrate the feasibility of growth of reasonable solar cells, the same is presented in chapter 5.