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Optical modeling of solar cells

Purnaansh P. Gunaicha

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A Thesis

Entitled

Optical Modeling of Solar Cells

By

Purnaansh P. Gunaicha

Submitted to the Graduate Faculty as partial fulfillment of the requirements for the

Master of Science Degree in Electrical Engineering

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The University of Toledo
December 2012
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An Abstract of
Optical Modeling of Solar Cells

By
Purnaansh P. Gunaicha

Submitted to the Graduate Faculty as partial fulfillment of the requirements for the Master of Science Degree in Electrical Engineering

The University of Toledo
December 2012

The fabrication of solar cells is a multi-stage process giving rise to a multitude of combinations of materials and cell parameters such as thickness, thin film growth conditions, ordering of layers and tandem cells. Experimentally investigating these combinations to optimize cell performance is expensive and time consuming. Computer simulations of the optical and electrical functions allow for eliminating large class of ineffective combinations and containing the parameter space significantly.

We modeled solar cell as a stack of layers. The wavelength dependent dielectric permittivity function defines the capacity of a material to absorb, reflect and transmit incident light. The light travels from one medium to another following simple principles and laws of reflection and refraction. Three important phenomena namely reflection, absorption and transmission take place at the interface of two layers in the cell structure. A coherent treatment of these phenomena using the incoming and outgoing and reflected electric field in each layer can be done. This approach yields the electric field at any point in each layer thereby helping in calculating the absorbed photons in the layer eventually allowing us to calculate the quantum efficiency (Q.E) and overall reflectance (R) and
transmittance (T) of the solar cell. The Q.E. allows the calculation of the short circuit current generated by the solar cell and the R and T allow for the calculation of the reflection loss of the solar cell. The analytical tool used in this thesis is based on such an approach and is used to evaluate the compatibility of the different materials with each other for being used in the solar cell.

We used different combinations of Transparent Conductive Oxides (TCOs’) for the solar cells analyzed in the work. The major focus of the thesis is to evaluate the dependence of the optical performance of the solar cell on the thickness of the layers of the solar cell along with different TCOs’. The solar cells considered in the work are Copper-Indium-Diselenide (CuInSe$_2$) and Copper-Indium-Gallium-Diselenide (CIGS, CuInGaSe$_2$).

The analysis of CuInSe$_2$ and CuInGaSe$_2$ showed that maximum current is produced when Indium – doped tin oxide (ITO) is used as TCO. The use of ITO as TCO results in highest short circuit current density for both the structures. The combination of Zinc Oxide (ZnO) and Aluminium-doped-Zinc Oxide (ZnO:Al) leads to lowest short circuit current density and highest reflection loss. The use of CuInSe$_2$ produces a high current compared to CuInGaSe$_2$. 
Dedicated to the support and motivation from my family and friends

“God helps those who help themselves”

Aesop’s Fables
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List of Abbreviations

λ …………………… Wavelength (nm)

CIS ………………… Copper Indium Diselenide
CIGS ………………. Copper Indium Gallium Diselenide
\( J_{SC} \) …………… Short Circuit Current Density (mA/cm\(^2\))
\( V_{OC} \) …………… Open Circuit Voltage (Volts)
ITO …………………….. Indium – doped – Tin Oxide
ZnO …………………… Zinc Oxide
ZnO:Al ……………….. Aluminum – doped – Zinc Oxide
CdS …………………… Cadmium Sulfide
Chapter 1

Introduction

Energy is defined as the capacity of a system to do work. As stated by the law of conservation of energy, “Energy can neither be created nor be destroyed; it can be transformed from one form to another. The total energy is constant.” (David Halliday, 1978) It can be obtained from different sources classified as “renewable and non-renewable energy sources.” The names are self-explanatory. Non-renewable energy sources will finish if their rate of usage is more than the rate of formation, example coal, natural gas. Renewable energy sources on the other hand are the “ever-lasting” sources of energy, example sunlight, wind. The non-renewable sources are cheap but the side-effects have been enormous on the environment which has made them unsustainable. The renewable sources example sunlight, have proven to be sustainable.

Sun’s light energy can be harnessed and be transformed into electricity with the help of solar-cells. The solar cells absorb the photons of the light from the sun and this absorption results in the build-up of a voltage due to the movement of the high energy electrons within the material which results in the production of electricity from them. The first solar cell was developed in 1954 at Bell laboratories but the cost of production of electricity was very high compared to the cost of electricity production using fossil fuels.
Over the years, the research in this field has taken its own course with breakthroughs in the improved efficiency, reduced cost and use of non-hazardous materials.

1.1 Solar cell

A typical solar cell is shown in Figure 1-1 (Manager, 2008):

![Figure 1-1 Cross Section of a solar cell (Stuart Bowden, Solar Cell Structure, 2010)](image)

The structure of the solar cell consists of:

a) Substrate – It forms the base on which the solar cell is constructed. The commonly used substrate is soda-lime-glass. The use of soda-lime-glass substrate improved the device performance which was attributed to the better match of thermal expansion coefficients. A more important effect on the device
performance was due to the diffusion of sodium from the glass to absorber. (Lundberg, 2003)

b) Absorber Layer – It is the layer where photons from sunlight are absorbed and charge carriers are generated. The material used for this layer should exhibit high absorption coefficients. Figure 1-2 shows the absorption coefficients of the different materials used for the absorber layer in the solar cells.

![Absorption Coefficients](image)

Figure 1-2 The absorption coefficient, $\alpha$, in a variety of semiconductor materials at 300K as a function of the vacuum wavelength of light (Stuart Bowden).

c) Transparent Conducting Oxide (TCO) – This forms the front-contact of the solar cell. The name itself suggests that the material should be transparent and conductive to allow for the unrestricted flow of the electrons. A few of TCOs’ are Indium-Tin-Oxide (ITO) and aluminum doped zinc oxide (ZnO:Al).

d) Back contact – This layer should be conductive, highly reflective and should not allow for any recombination of holes and electrons. The material should be inert
and nonreactive during the absorber deposition process. Molybdenum has been the best available material to be used for back contact, also allowing the sodium to diffuse from glass to the absorber layer.

e) Buffer layer – This layer assists in the formation of the pn-junction which would be responsible for generation of charge carriers which eventually contribute to the current generated by the solar cell. The effect of this layer on the device performance is not completely understood. Cadmium Sulfide (CdS) is the most common. The incomplete understanding of the function of this material used in the layer has proven to be a difficulty in replacing it by a non-toxic material.

1.2 Motivation

Coal, oil and natural gas have become a very important portion of lives. The technologically advanced world will slow down in its progress if these resources run-out and we are in-fact running out of these resources. The increasing population of the world, which has led to increased demand and consumption of these resources, is leading fast towards their extinction. Their cost has increased significantly as they are becoming scarcer. These resources have also added to air pollution, depletion of ozone layer, increased formation of the greenhouse gases, polluting the water bodies. The high pollution, increased rate of consumption and our dependability on them requires us to make ourselves ready for the time when they will vanish from the earth.

The renewable sources provide a solution to all our problems. They are abundant and everlasting, example sunlight, wind. They do not have adverse effects on the
environment. Their utilization is costly right now but a thorough research will have its own breakthroughs.

The solar cells trap sunlight and generate electricity. The more the number of photons absorbed by the absorber layer, more electricity will be generated. The common basis of highly-efficient and cost-effective production of electricity requires us to look into improving different aspects of a solar cell structure. An efficient conversion of sunlight to electricity can be achieved if the following factors are considered in the design of a solar cell:

a) Use of material with high absorption coefficient for the absorber layer.

b) Highly conductive TCO.

c) Reflective back contact to allow more light to be passed through the absorber layer.

d) Optimum thickness of the different layers of the solar cell to provide maximum absorption in the absorber, least reflectance and transmittance from the cell and a cost-effective production of electricity.

e) Non-recombination of electrons and holes in the back contact layer.

f) Assuring a smooth travel and collection of the electrons for higher electricity generation.

g) Use of abundant and non-toxic materials for all the layers of the cell.

The focus of the thesis is to explore the possibilities of combining different materials for the layers of a solar cell and calculation of the optimum thickness of these
layers with the objective of higher absorption in the absorber layer, less reflection and transmittance and cost-effective manufacturing of the cell.

1.3 Thesis outline

The thesis is based on the optical modeling of the solar cell. The analysis is subdivided into the following:

Chapter 2 discusses the theory and the physics underlying the optical modeling of the solar cell and the analytical tool developed for the same.

Chapter 3 and Chapter 4 constitute the application of the tool on different solar cell structures and their results.

Chapter 5 explains the possible future work to obtain more accurate results from the tool.
Chapter 2

Optical Modeling

2.1 Overview

The development of the optical model serves the requirement of achieving the highest possible absorbance in the absorber layer thereby minimizing the absorbance in the other layers and the optimum thickness of each layer to make the cell manufacturing cost-effective. The solar cell is represented as a stack of layers consisting of the front and back contact, absorber layer, substrate and buffer layer in their respective positions is shown in Figure 1-1. The theory underlying the model is based on the model present in the paper Leif A. A. Pettersson, Lucimara S. Roman, and Olle Inganäs. The model utilizes the complex dielectric constants calculated experimentally using the spectroscopic ellipsometry technique. These constants are calculated for a number of different wavelengths. The absorbance in different layers of the cell is calculated by evaluating the distribution of electric field in the layers. The electric fields are evaluated using the complex Fresnel’s coefficient of reflection and transmission for the layer which in-turn are calculated using the matrix approach. The output is the absorbance in each layer of the solar cell, the overall reflectance and transmittance of the cell. The output is used to calculate the short circuit current, reflection and transmission loss for the structure by integrating them over the desired spectral range, visible spectrum in our case. The standard photon flux used for the calculation is the AM1.5.
2.2 Input

The dielectric constants ($\varepsilon_1$ and $\varepsilon_2$) of the different layers of the solar cell and the thickness of the layers under experiment are obtained by spectroscopic ellipsometry (SE). The constants are in a file format which is input for the model. The structure of the solar cell is defined in a master file along with the thicknesses of different layers.

Five approaches have been adopted for application of SE to alloy materials and device development: (1) Ex-situ SE has been performed on as-deposited films to determine the band gap and critical point structure (i.e., the higher energy band gaps). Such measurements can also be repeated after post-deposition treatments (such as annealing in chloride vapor) and the energy shifts and changes in width of the band gap and critical point structures provide information on the survivability and ultimately the improvement of the alloy (Parikh A.). (2) Accurate dielectric functions have been obtained for those alloys that have been successfully treated post deposition while retaining the appropriate composition of the alloy and its band gap. Dielectric functions have also been determined for all other device components, including the glass (Chen, 2006), transparent top and back contact, interconnect junction, and metal contact materials. (3) the Bruggeman effective medium approximation, is used to determine optical properties of interface layer assuming a composite of the overlying and underlying materials (4) the built-in data base provided by J.A.Woollam has been used for those materials for which ex-situ ellipsometry is not performed (5) Finally, the dielectric function database has been used in the optical design of single-junction and multi-junction solar cell structures. For multi-junction configuration current matching
condition is satisfied for optical analysis. In such studies, the maximum possible current is determined, based on incident AM1.5 irradiance.

2.3 Computation technique

The assumptions in the model are (Leif A. A. Pettersson, 1999):

a) The layers of the device are homogeneous and isotropic. This help in utilizing the scalar complex index of refraction to describe their optical response.

b) The interfaces between the layers are parallel and smooth. The surfaces are not “rough” but flat.

c) The incident light can be described by plane waves.

b) All the generated charges contribute to the photocurrent implying that none of the charges are trapped inside the device.

According to (Bashar, 1977) the reflection and transmission behavior of a set of stacked layer/s on the top of a substrate with different materials and/or different compositions can be described using the 2x2 matrices (S matrix). This is possible because the equations governing the propagation of electric field are linear and tangential component of the electric field is continuous (Leif A. A. Pettersson, 1999).

Assume the light incident on a stratified structure Figure 2-1 from left with a semi-infinite ambient, indexed 0, propagating through the structure to the semi-infinite substrate, indexed, m+1. The entire structure can be represented by the S matrix written as:

\[ S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} = \left( \prod_{v=1}^{m} l(v-1)vL_v \right) L_{m(m+1)} \quad (1) \]
Where the interface matrix at the interface “j/k” is defined as:

\[
I_{jk} = \frac{1}{t_{jk}} \begin{bmatrix} 1 & r_{jk} \\ r_{jk} & 1 \end{bmatrix}
\]  

(2)

Where \(r_{jk}\) and \(t_{jk}\) are the complex Fresnel reflection and transmission coefficients respectively at the interface j/k.

Figure 2-1 The general stratified structure between a semi-infinite ambient and semi-infinite substrate. The layers are numbered from 1,2,3...m; m+1 being the substrate and ambient being 0. The thickness of a layer is designated as \(d_j\). The electric field at any point in the layer is defined by two components, one in positive direction \(E_j^+\) and one in the negative direction \(E_j^-\).

The Fresnel coefficients of reflection and transmission at the interface j/k for the light with electric field perpendicular to the plane of incidence (TE wave) are respectively defined as:

\[
r_{jk} = \frac{(n_j \cos \phi_j - n_k \cos \phi_k)}{(n_j \cos \phi_j + n_k \cos \phi_k)}
\]  

(3)

And
Similarly, the Fresnel coefficients of reflection and transmission for the light with electric field parallel to the plane of incidence (TM wave) are respectively defined as:

\[ t_{jk} = \frac{2n_j \cos \phi_j}{(n_j \cos \phi_j + n_k \cos \phi_k)} \]  

(4)

And

\[ r_{jk} = \frac{(n_k \cos \phi_j - n_j \cos \phi_k)}{(n_k \cos \phi_j + n_j \cos \phi_k)} \]  

(5)

Where \( n_x \) is the complex index of refraction for the layer “x”, \( \phi_j \) is the angle of refraction in the layer “j” and \( \phi_k \) is the angle of refraction in the layer “k”. The layer matrix \( L_j \) describing the light propagation through the layer “j” is:

\[
L_j = \begin{bmatrix}
e^{i \xi_j d_j} & 1 \\
1 & e^{-i \xi_j d_j}
\end{bmatrix}
\]  

(7)

Where;

\[ \xi_j = \frac{2 \pi n_j \cos \phi_j}{\lambda} \]  

(8)

Where the product \( \xi_j d_j \) represents the change in the phase of the wave when it traverses through a layer with thickness \( d_j \).

Thus the electric field on the ambient side can be related to the electric field on the substrate side using the scattering matrix as follows:

\[
E = \begin{bmatrix} E_0^+ \\ E_0^- \end{bmatrix} = S \begin{bmatrix} E_{m+1}^+ \\ E_{m+1}^- \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} E_{m+1}^+ \\ E_{m+1}^- \end{bmatrix} \]  

(9)

Since the wave is incident from ambient side in the positive x-direction there is no wave propagating in the negative x-direction inside the substrate, which means \( E_{m+1}^- = 0 \).
Therefore, for the stratified structure the overall complex reflection and transmission coefficients can be expressed as:

\[ r = \frac{E_0^-}{E_0^+} = \frac{S_{21}}{S_{11}} \]  
\[ (10) \]

\[ t = \frac{E_{m+1}^+}{E_0^+} = \frac{1}{S_{11}} \]  
\[ (11) \]

In order to calculate the electric field in the layer “j” the stratified structure can be divided into two portions separated by the layer “j”. The total system transfer matrix S can then be represented as:

\[ S = S' \mathbf{L}_j S'' \]  
\[ (12) \]

Where \( S'_j \) and \( S''_j \) are the partial system transfer matrices separated by the layer j, defined as:

\[ \begin{bmatrix} E_0^+ \\ E_0^- \end{bmatrix} = S'_j \begin{bmatrix} E_j^+ \\ E_j^- \end{bmatrix} = \begin{bmatrix} S'_{j11} & S'_{j12} \\ S'_{j21} & S'_{j22} \end{bmatrix} \begin{bmatrix} E_j^+ \\ E_j^- \end{bmatrix} \]  
\[ (13) \]

Where \( S'_j \) is the system transfer matrix for the system to the left of the layer “j” and \( E_j^+ \) and \( E_j^- \) refer to the fields on the left boundary of the layer “j”.

\[ \begin{bmatrix} E_j'^+ \\ E_j'^- \end{bmatrix} = S'' \begin{bmatrix} E_{m+1}^+ \\ E_{m+1}^- \end{bmatrix} = \begin{bmatrix} S''_{j11} & S''_{j12} \\ S''_{j21} & S''_{j22} \end{bmatrix} \begin{bmatrix} E_{m+1}^+ \\ E_{m+1}^- \end{bmatrix} \]  
\[ (14) \]

Where \( S''_j \) is the system transfer matrix for the system to the right of the layer “j” and \( E_j'^+ \) and \( E_j'^- \) refer to the fields on the right boundary of the layer “j”.

Similar to the Fresnel coefficients for the whole stratified structure these coefficients can be defined for the partial systems \( S'_j \) and \( S''_j \).
Combining the Eq. (10) – (18) the electric field propagating in the positive x-direction in the layer “j” can be described as:

\[ E_j^+ = \frac{t_j^'}{1 - r_j^'-r_j^''e^{i2\xi_jd_j}} E_0^+ \]  

(19)

Where \( r_{j'} = -\frac{s_{j12}}{s_{j11}} \). Similarly the electric field propagating in the negative x-direction in the layer “j” can be related to the incident electric field as:

\[ E_j^- = \frac{t_j^'r_j^''e^{i2\xi_jd_j}}{1 - r_j^'-r_j^''e^{i2\xi_jd_j}} E_0^+ \]  

(20)

The total electric field in the layer “j” at a distance “x” to the right of the boundary \((j - 1)j\) in terms of the incident electric field is given by:

\[ E_j(x) = E_j^+(x) + E_j^-(x) \]  

(21)

The term \( d_j \) in Eq. (19) will be replaced by \( x \) and the same term \( d_j \) in Eq. (20) will be replaced by \((d_j - x)\) where \( 0 \leq x \leq d_j \).
2.4 Output

The computed electric field is utilized to calculate the absorbance in the layer which helps in calculating the quantum efficiency, photocurrent/short circuit current. The definitions and the calculation steps constitute the next sections of the chapter.

2.4.1 External Quantum Efficiency

External quantum efficiency (E.Q.E.) is defined as the ratio of the number of carriers absorbed by the solar cell to the number of photons of a given wavelength/energy incident on the cell. The quantum efficiency equals unity if all the incident photons at a particular wavelength are absorbed and all the resulting minority carriers are collected. The E.Q.E. for photons with energy below the band gap is zero. The external quantum efficiency curve is shown in Figure 2-2 (Stuart Bowden):

![External Quantum Efficiency Curve](image)

Figure 2-2 The external quantum efficiency curve. The rectangle is the ideal curve. The figure shows the E.Q.E. curve for a silicon solar cell.
The Poynting vector (F. Leblanc, 1994) $\mathbf{\Sigma}$ correlates the total electromagnetic field with the electromagnetic energy transport through the stack. Its flux through a unit area of interface surface is the power flux passing through this surface. $\mathbf{\Sigma}$ is given by

$$\mathbf{\Sigma} = \frac{1}{2} \text{Re}[\mathbf{E} \times \mathbf{H}^*]$$

where $\text{Re}$ ($\text{Im}$) refers to the real (imaginary) part of a complex vector, and $^*$ to the conjugation operator.

The absorptance $A_j$ in any layer ($j$) is obtained by taking the difference of the power flux through the top interface and the bottom interface of the layer as follows,

$$A_j = \frac{\Sigma_{\text{top}} - \Sigma_{\text{bottom}}}{\Sigma_{\text{inc}}}$$

In the case of normal incidence, flux in TE mode and TM mode is same and hence calculation of absorptance is simple subtraction from of top and bottom flux when incident flux is normalized to one.

Please note that henceforth the terms External Quantum Efficiency (EQE) and Quantum Efficiency (QE) would be used interchangeably. Both the terms refer to the External Quantum Efficiency (EQE).

### 2.4.2 Spectral Irradiance

The spectral irradiance (Stuart Bowden) provides the power density of the photon of a particular wavelength. The units of spectral irradiance are in $\text{Wm}^{-2}\mu\text{m}^{-1}$ i.e. power density of $\text{Wm}^{-2}$ at the wavelength $\lambda$ ($\mu\text{m}$). Therefore, the $\text{m}^{-2}$ refers to the surface area of the light emitter and the $\mu\text{m}^{-1}$ refers to the wavelength of interest.
In the analysis of solar cells, the photon flux is often needed as well as the spectral irradiance. The spectral irradiance can be determined from the photon flux by converting the photon flux at a given wavelength to Wm\(^{-2}\). The result is then divided by the given wavelength, as shown in the equation below.

\[
F = \left( \frac{W}{m^2 \mu m} \right) = q\Phi \frac{1.24}{\lambda^2(\mu m)} = q\Phi \frac{E^2(eV)}{1.24}
\]

Where:

- \(F\) is the spectral irradiance in W\(m^{-2}\)\(\mu m^{-1}\);
- \(\Phi\) is the photon flux in number of photons m\(^{-2}\)sec\(^{-1}\);
- \(E\) and \(\lambda\) are the energy and wavelength of the photon in eV and \(\mu m\) respectively; and
- \(q, h \text{ and } c\) are constants.

### 2.4.3 Photon Flux

The photon flux (Stuart Bowden) is defined as the number of photons per second per unit area:

\[
\Phi = \frac{\text{number of photons}}{\sec m^2}
\]

The photon flux is an important quantity in calculation of the current generated from the cell. The flux is independent of the wavelength (or energy) of the photons, therefore the wavelength at which the flux is calculated must be associated with it. Since the photon flux gives the number of photons striking a surface in a given time, multiplying by the energy of the photons comprising the photon flux gives the
energy striking a surface per unit time, which is equivalent to a power density. To
determine the power density in units of Wm\(^{-2}\), the energy of the photons must be in
Joules. The equation is:

\[
H \left( \frac{W}{m^2} \right) = \phi \cdot \frac{hc}{\lambda} \cdot J = q\phi \cdot \frac{1.24}{\lambda(\mu m)}
\]

Where: \(\phi\) is the photon flux.

2.4.4 Short Circuit Current Density from External Quantum Efficiency

The photocurrent generated by a solar cell under illumination at short circuit
depends on the incident light.

\[
J_{sc} = q \int b_s(\lambda) \cdot EQE(\lambda) d\lambda
\]

Where

- \(q\) – magnitude of one electronic charge.
- \(b_s(\lambda)\) – Incident spectral photon flux density for photon of wavelength \(\lambda\).
- \(EQE(\lambda)\) – External Quantum Efficiency for photon of wavelength \(\lambda\).

Please note that henceforth the terms “short circuit current density” and “current” will be
used interchangeably. The terms will refer to short circuit current density (mA/cm\(^2\)).

2.4.5 Reflectance /Transmittance

The probability that the sunlight consists of s-wave and p-wave is fifty-fifty
respectively. This means 50% of the incident photons can be considered to behave like s-
waves and the remaining 50% of the incident photons can be considered to behave like p-wave. The reflectance therefore will have equal contributions from the complex Fresnel coefficient of reflection for s-wave and p-wave which can be represented as

\[ R = \frac{1}{2} \left( R_p + R_s \right) \]

Where

\[ R_p = r_p^2 \]

And

\[ R_s = r_s^2 \]

Similar arguments hold for the overall transmittance of the stratified structure:

\[ T = \frac{1}{2} \left( T_p + T_s \right) \]

Where

\[ T_p = t_p^2 \]

And

\[ T_s = t_s^2 \]

The reflectance and transmittance for the desired range of wavelength are used to evaluate the loss due to reflection and transmission from the solar cell. The procedure followed is similar to the calculation of photocurrent from quantum efficiency.
Chapter 3

Copper-Indium-Diselenide (CuInSe$_2$) Solar cell

The synthesis and characterization of Copper-Indium-Diselenide (CuInSe$_2$/CIS) was first reported by Hahn in 1953 (Hahn, 1953). The first CuInSe$_2$ solar cells were made by (Wagner S, 1974) using p-type single crystals of CuInSe$_2$ and evaporating n-type Cadmium Sulfide (CdS) on them. The early solar cells were reported to exhibit an efficiency of 12% “on a clear day in New Jersey” (Shay J, 1975). There was reduced focus on devices using single crystal CuInSe$_2$ due to the difficulty of growing high quality crystals. The focus was moved towards fabricating thin film CuInSe$_2$/CdS due to their inherent advantages. Kazmerski et al. were the first group to report the thin film solar cells based on CuInSe$_2$/CdS by using of evaporation CuInSe$_2$ powder along with excess Se to deposit their films (Kazmerski L, 1976).

It was in 1981 when Boeing demonstrated high-efficiency (9.4%) CuInSe$_2$/CdS thin film solar cell. These devices used co-evaporation to fabricate their films of CuInSe$_2$ on ceramic substrates which were coated with molybdenum back electrode (Mickelsen R, 1982). These devices were then coated with evaporated CdS deposited in two layers with undoped-CdS followed by In-doped-CdS which acted as the main current carrying material (Mickelsen R, 1982).
The CuInSe$_2$/CdS solar cell technology was boosted when Boeing and ARCO Solar began to address the issues relating to scale up, efficiency and throughput (Antonio Luque, 2003). Soda lime glass replaced the ceramic glass substrate which resulted in increased device performance and process tolerance (Hedstrom, 1993). The doped CdS layer was thinned from 1-2μm to undoped layer of 50nm and less. A conductive ZnO current carrying layer was added to the undoped CdS layer (Potter, 1986).

CuInSe$_2$ has been considered a promising material for fabricating thin film solar cells because of its favorable properties such as direct band gap, high absorption coefficient. Along with the advancement of technology it became apparent that CuInSe$_2$ could be used with wide compositions by introducing “Ga” which eventually led to the development of the material (Copper-Indium-Gallium-Diselenide) CuInGaSe$_2$.

### 3.1 Material properties

CuInSe$_2$ is direct band gap material with high absorption coefficient existing in the chalcopyrite lattice structure. The lattice constants $a$ and $c$ for CuInSe$_2$ are $5.78\text{Å}$ and $11.62\text{Å}$ producing the $c/a$ ratio $\approx 2.01$ (Suri D, 1989). The dielectric constants at low and high frequency are reported to be $13.6 \pm 2.4$ and $8.1 \pm 1.4$ respectively (Wasim, 1986). The band gap of CuInSe$_2$ is 1.02eV (Neumann, 1986). Figure 3-1 shows the dielectric constants of the CuInSe$_2$ material used in the calculations. Table 3.1 summarizes some of the selected properties of CuInSe$_2$. 

![Figure 3-1](image_url)
Table 3.1 Properties of CuInSe$_2$

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Units</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lattice Constant (a,c)</td>
<td>5.78, 11.62</td>
<td>Å</td>
<td>(Suri D, 1989)</td>
</tr>
<tr>
<td>Density</td>
<td>5.75</td>
<td>g/cm$^3$</td>
<td>(Suri D, 1989)</td>
</tr>
<tr>
<td>Melting Temperature</td>
<td>986</td>
<td>Celsius</td>
<td>(Ciszek, 1984)</td>
</tr>
<tr>
<td>Thermal expansion coefficients at 273 K</td>
<td>8.32 x 10$^{-6}$</td>
<td>1/K</td>
<td>(Neumann, 1986)</td>
</tr>
<tr>
<td>(a-axis, c-axis)</td>
<td>7.89 x 10$^{-6}$</td>
<td>1/K</td>
<td></td>
</tr>
<tr>
<td>Thermal conductivity at 273 K</td>
<td>0.086</td>
<td></td>
<td>(Neumann, 1986)</td>
</tr>
<tr>
<td>Energy gap</td>
<td>1.02</td>
<td>eV</td>
<td>(Neumann, 1986)</td>
</tr>
<tr>
<td>Energy Gap temperature coefficient</td>
<td>-2 x 10$^{-4}$</td>
<td>eV/K</td>
<td>(Neumann, 1986)</td>
</tr>
</tbody>
</table>

Figure 3-1 Optical constants of CuInSe$_2$

The dielectric constant $\varepsilon_2$ is zero below the value of ~ 0.85eV which suggests that the band gap of the CuInSe$_2$ used in the study is ~ 0.85eV. This band gap is lower compared to the ideal band gap because of the difference in the environment and the process with which the thin film of CuInSe$_2$ has been fabricated.
3.2 Optical Analysis

The analysis focuses on the dependence of the optical parameters such as quantum efficiency, reflectance and transmittance of a solar cell on the thickness of its constituent layers. The dielectric constants; obtained experimentally, of different materials in the solar cell structure are provided as the inputs to the program. The solar cell used in the study is CIS (Copper Indium DiSelenide) solar cell. Table 3.2 shows the general structure of CuInSe₂ solar cell.

Table 3.2 General substrate model of CuInSe₂ solar cell

<table>
<thead>
<tr>
<th>TCO (Transparent Conductive Oxide)</th>
<th>CdS (Buffer Layer)</th>
<th>CIS (Absorber or Active layer)</th>
<th>Molybdenum (Back Contact)</th>
<th>Soda Lime Glass (Substrate)</th>
</tr>
</thead>
</table>

The TCO layers in the above solar cell have been used in different combinations:

1) ZnO with Al-doped-ZnO

2) ZnO with ITO (Indium – doped – Tin Oxide)

3) Indium – doped – Tin Oxide (ITO)

For each of the combination of TCOs, the thickness dependence study of the optical properties of solar cell is carried out. This is performed in the following manner:

1) Thickness variation of Absorber Layer – The thickness of the absorber layer is varied and the thickness of the other layers is kept constant to get the optimum
value of the absorber thickness which provides for increased current and reduced reflection loss.

2) Thickness Variation of the TCO – The TCO thickness is varied in the following way:

   a. If the TCO is a combination of two compounds then the thickness of each layer is varied and its effect on the optical properties of solar cell is observed and the best thickness is reported. For Eg: In a combination of ZnO and Al-doped-ZnO, the thickness of Al-doped-ZnO is varied initially and then, after selecting the optimal thickness of Al-Doped-ZnO the thickness of ZnO layer is varied to report the optimum value of the thickness of the layer.

   b. If TCO is only a single compound then the thickness of the layer is varied and the best thickness is reported.

3) Thickness Variation of Buffer Layer – The thickness of the buffer layer (CdS) is varied and its effect on the absorbance, reflectance and transmittance of the solar cell is studied and the optimum thickness is then reported.

4) Thickness Variation of Back Contact – After having the optimum values of the thicknesses of the absorber layer, TCO’s and buffer layer; the dependence of the optical properties on the thickness of the back contact (Molybdenum) layer is studied.

The chapter is divided into the following sections

1) Solar cell structure with TCO as a combination of ZnO and Al-doped-ZnO

   a. Thickness variation of the absorber layer
b. Thickness variation of the Al-Doped-ZnO layer  
c. Thickness variation of the ZnO layer  
d. Thickness variation of the buffer (CdS) layer  
e. Thickness variation of the back contact (molybdenum)  
f. Optimal structure of the solar cell  

2) Solar cell structure with TCO as a combination of ZnO and ITO  
a. Optimal structure of the solar cell  

3) Solar cell structure with TCO as ITO only  
a. Optimal structure of the solar cell  

4) Comparison of the three structures of CIS solar cell  

3.3 Solar cell structure with TCO as a combination of ZnO and Al–Doped–ZnO  

Table 3.3 shows the structure of the solar cell used for the study.  

Table 3.3 Substrate model of CuInSe₂ solar cell  

<table>
<thead>
<tr>
<th>Al – Doped – ZnO</th>
</tr>
</thead>
<tbody>
<tr>
<td>ZnO</td>
</tr>
<tr>
<td>CdS</td>
</tr>
<tr>
<td>CIS</td>
</tr>
<tr>
<td>Molybdenum</td>
</tr>
<tr>
<td>Soda lime glass</td>
</tr>
</tbody>
</table>

3.3.1 Thickness variation of the absorber/active layer  

The thickness of the absorber layer (CIS) of the solar cell is varied while keeping the thicknesses of the other layers constant. The thickness variation of the cell is mentioned in Table 3.4:
Table 3.4 Substrate model of CuInSe₂ solar cell with thickness variation of the absorber layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>3.0×10⁶</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>4.0×10⁻⁷</td>
</tr>
<tr>
<td>CIS</td>
<td>5.0×10⁻² – 5.0×10⁻³</td>
</tr>
<tr>
<td>CdS</td>
<td>50</td>
</tr>
<tr>
<td>ZnO</td>
<td>60</td>
</tr>
<tr>
<td>Al – Doped – ZnO</td>
<td>120</td>
</tr>
</tbody>
</table>

The quantum efficiency of the absorber layer of the solar cell for the thickness of interest is shown in Figure 3-2.

The quantum efficiency (Q.E.) is measured from 305 nm – 1490 nm. The Q.E. is generally not measured below 350 nm due to the low power contained in the AM1.5 at such low wavelengths (Stuart Bowden).

The quantum efficiency at lower wavelengths i.e. 300 nm-500 nm is found to be low due to higher absorption in the TCO layers and the buffer layer. The photons of higher energies are absorbed by the TCO and buffer layer.

The mid-energy photons i.e. 500 nm ≤ λ ≤ 1300 nm are absorbed highly in the absorber layer because their energy levels are too-high/too-low to be absorbed by other layers. The photons lie beyond/below the band gap of the other layers which does not permit them to be absorbed. These photons are either absorbed by the absorber layer or reflected back by the cell.
Figure 3-2 Quantum efficiency of the active layer of CuInSe$_2$ solar cell. The graph is shown for different thickness of the absorber layer.

The low energy photons i.e. wavelength ($\lambda$) $> 1490$ nm have energy lower than the band gap of the absorber layer and thus are not absorbed by it. The steep fall while approaching the higher wavelength range i.e. $1300$ nm $\leq \lambda \leq 1490$ nm can be explained due to increased reflection from the solar cell. Recombination in the back contact layer can also be one of the reasons for the fall in the Q.E.

The thickness dependence of the Q.E. shows that it increases with the increase in the thickness of the absorber layer but tends to reach a saturation point beyond which the absorption is non-substantial. The thickness beyond which this saturation is observed is chosen to be the optimal thickness of the active layer.
The dependence of reflectance of the solar cell on the wavelength of light is shown in Figure 3-3. The reflection from the solar cell is low for wavelength ($\lambda \leq 1300$ nm) due high absorbance within the solar cell. The lower energy photons are least absorbed by the solar cell leading to a high rate of reflection from the solar cell. The reflectance shows a trend similar to the Q.E. i.e. increased reflection with increased thickness of the absorber layer. Some of these photons may be absorbed due to recombination in the back contact of the solar cell. The rest of the photons are reflected back into the atmosphere.

![Figure 3-3 Reflectance of the solar cell. The graph is shown for different thickness of the absorber layer.](image-url)
The current and reflection loss are computed by integrating the product of the optical absorbance and AM 1.5 spectral photon flux over the spectral range from 305 nm to 1490 nm. This range of wavelength is chosen to cover the whole range for absorption of the photons by the absorber layer. Figure 3-4 shows the dependence of the current and the reflection loss of the solar cell on the thickness of the absorber layer.

The current in the solar cell is produced due to the photons absorbed in the absorber layer. The current is found to increase with the increase in the thickness of the absorber layer and the reflection loss decreases with increase in the absorber layer thickness. The current and the loss tend to become “independent/un-affected” due to the increase in the thickness of the layer after the point of 2 μm. They reach the point where a minor increase in the thickness does not lead to a major increase/decrease in the current/loss. Thus the intended thickness of the absorber layer is chosen to be 2 μm.
3.3.2 Thickness variation of the Al – Doped ZnO Layer

The thickness of the Al-doped-ZnO (ZnO:Al) layer, which forms a portion of the TCO is varied in this section. The thickness of the other layers is kept constant. Table 3.5 shows the structural thickness variation of the cell.
Table 3.5 Substrate model of CuInSe₂ solar cell with the thickness variation of Al-doped-ZnO layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>3.0×10⁶</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>4.0×10⁻²</td>
</tr>
<tr>
<td>CIS</td>
<td>2.0×10⁴</td>
</tr>
<tr>
<td>CdS</td>
<td>50</td>
</tr>
<tr>
<td>ZnO</td>
<td>60</td>
</tr>
<tr>
<td>Al–Doped–Zno</td>
<td>60 – 180</td>
</tr>
</tbody>
</table>

The Q.E. of Al-doped-ZnO and the absorber layer is shown in Figure 3-5. The comparison of the two curves in Figure 3-5 allows us to infer the effect of the thickness variation of the ZnO:Al layer on the Q.E. of the absorber layer.
Figure 3-5 Comparison of the quantum efficiency of the ZnO:Al (top) with the quantum efficiency of absorber (bottom) for different thickness of ZnO:Al.

The Q.E. of the two layers in Figure 3-5 is compared for the wavelength (λ) range 305 nm ≤ λ ≤ 1490 nm. The spectral range of Q.E. can be divided into different regimes; (a) 305 nm ≤ λ ≤ 500 nm, (b) 500 nm ≤ λ ≤ 1300 nm, (c) 1300 nm ≤ λ ≤ 1490 nm, (d) λ ≥ 1490 nm.

As seen in Figure 3-5 the low Q.E. of the active layer in the low wavelength range, 305 nm ≤ λ ≤ 500 nm, is a result of high absorption taking place in the ZnO:Al layer which gradually decreases while approaching the 500 nm mark. Consequently, an increase in the Q.E. of the active layer can be seen resulting in increasing absorption of high energy photons.
The Q.E. of the active layer keeps on increasing and reaches its maximum in the wavelength range, $500 \text{ nm} \leq \lambda \leq 1300 \text{ nm}$. This is primarily due to the energy of the photons falling beyond/below the band gap energy of other layers. This high absorption is reflected in the low reflectance from the solar cell for the particular wavelength range.

There is a steep fall in the high wavelength range $1300 \text{ nm} \leq \lambda \leq 1490 \text{ nm}$ for the solar cell. This is due to increasing absorption in the ZnO:Al as well as the recombination taking place in the back contact layer. These photons fall beyond the band gap energy of the TCO and buffer layer. This allows for the reflection of these photons from the solar cell.

The photons for wavelength $\lambda \geq 1490 \text{ nm}$ fall beyond the band gap of the TCO, buffer layer and active layer leading to their least absorption. They are reflected back into the atmosphere. The thickness dependence of the Q.E. of the active layer shows a trend of increasing with the decrease in the thickness of the ZnO:Al layer. The thickness reduction of the ZnO:Al has a considerable effect on the Q.E. of the active layer.

The dependence of the reflectance of the cell on the wavelength is shown in Figure 3-6. It is not affected by the variation in thickness of ZnO:Al in the wavelength range $305 \text{ nm} \leq \lambda \leq 900 \text{ nm}$. It shows a trend of increasing with the increase in the thickness of ZnO:Al for the higher wavelengths/lower energies. The solar cell requires low reflectance to allow for more absorption in the active layer. The thickness of ZnO:Al is reduced to 75 nm so that it does not affect the absorption in active layer as well as there is reduced reflectance from the solar cell.
As shown in the previous section, the current and reflection loss are computed by integrating the product of the optical absorbance and AM 1.5 spectral photon flux over the spectral range from 305 nm to 1490 nm. This range of wavelength is chosen to cover the whole range for absorption of the photons by the absorber layer. Figure 3-7 shows the dependence of the current and the reflection loss of the solar cell on the thickness of the absorber layer.

The current in the active layer is found to decrease with the increase in the thickness of the ZnO:Al layer and the reflection loss increases (it does not follow a particular trend for the whole range but shows the increasing trend for wavelength range of interest) with increase in the thickness of the ZnO:Al. The current and the loss do not change in considerable amounts with minor changes in the thickness of ZnO:Al beyond
the point of 75 nm. Thus, 75 nm is the chosen thickness for the Al-doped-ZnO (ZnO:Al) layer of the CuInSe₂ solar cell.

![Graph of Current vs. Thickness](image)

![Graph of Reflection Loss vs. Thickness](image)

**Figure 3-7** Variation in the short circuit current density in the absorber layer with the thickness of Al-Doped-ZnO layer.

### 3.3.3 Thickness variation of the ZnO layer

The thickness of the ZnO layer, which forms the bottom portion of the TCO of the CuInSe₂ is varied in this section. The thickness of the other layers is kept constant. The variation of thickness is shown in Table 3.6:
Table 3.6 Structure of CuInSe\textsubscript{2} solar cell with thickness variation of ZnO layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>3.0×10\textsuperscript{6}</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>4.0×10\textsuperscript{4}</td>
</tr>
<tr>
<td>CIS</td>
<td>2.0×10\textsuperscript{3}</td>
</tr>
<tr>
<td>CdS</td>
<td>50</td>
</tr>
<tr>
<td>ZnO</td>
<td>30 – 140</td>
</tr>
<tr>
<td>Al – Doped – Zno</td>
<td>75</td>
</tr>
</tbody>
</table>

The Q.E. of the ZnO layer is shown in Figure 3-8 along with the Q.E. of the active layer which provides and insight to how the variation in the thickness of ZnO affects the Q.E. of ZnO which eventually affects the Q.E. of the active layer.

The Q.E. in Figure 3-8 is shown for the wavelength range 305 nm \( \leq \lambda \leq \) 1490 nm. As shown in the previous section the curve can be subdivided into subsections of smaller wavelength regimes: (a) 305 nm \( \leq \lambda \leq \) 500 nm, (b) 500 nm \( \leq \lambda \leq \) 1300 nm, (c) 1300 nm \( \leq \lambda \leq \) 1490 nm and (d) \( \lambda \geq \) 1490 nm.

In the spectral regime 305 nm \( \leq \lambda \leq \) 500 nm the Q.E. of the active layer is very low due to the increased absorption in the TCO. This can also be related to the high absorption in the ZnO:Al layer for the high energy photons. The reflectance is also reduced in this spectral range due increased absorption. The actual function of the TCO to allow unrestricted flow of carriers is restricted in this wavelength range.
The Q.E. of the active layer increases and reaches the maximum in the spectral range $500 \, \text{nm} \leq \lambda \leq 1300 \, \text{nm}$. This is due to the smaller band gap of the other materials used in the solar cell structure. The Q.E. should ideally be 1 in this spectral range but is reduced due to reflection from the cell and the low diffusion lengths of some of the carriers which should be absorbed but recombine before they can be used to add up to the flow of carriers in the active layer.

The Q.E. for the spectral range $1300 \, \text{nm} \leq \lambda \leq 1490 \, \text{nm}$ decreases with increase in the thickness of ZnO. This is due to the surface passivation in the rear. For the
wavelength \( \lambda \geq 1490 \text{ nm} \), the photons are not absorbed by the active layer as they fall out of the band gap of the same.

The reflectance of the solar cell with ZnO as TCO does not follow a particular trend for the whole wavelength range. It is found that for the wavelength range \( 800 \text{ nm} \leq \lambda \leq 1300 \text{ nm} \) it increases with increase in the thickness of ZnO layer but for wavelength \( \lambda \geq 1300 \text{ nm} \) it decreases with increase in the thickness of ZnO layer. These low energy photons are reflected back into the atmosphere.

![Figure 3-9 Reflectance of the solar cell.](image)

As shown in the earlier sections, the current and reflection loss are computed by integrating the product of the optical absorbance and AM 1.5 spectral photon flux over the spectral range from 305 nm to 1490 nm. This range of wavelength is chosen to cover the whole range for absorption of the photons by the absorber layer. Figure 3-10 shows
the dependence of the current and the reflection loss of the solar cell on the thickness of the absorber layer.

The current in the active layer is found to decrease with the increase in the thickness of the ZnO layer and the reflection loss increases (it does not follow a particular trend for the whole range but shows the increasing trend for wavelength range of interest) with increase in the thickness of the ZnO. The current and the loss do not change in considerable amounts with minor changes in the thickness of ZnO beyond the point of 60nm. Thus, 60nm is the chosen thickness for the ZnO (ZnO) layer of the CuInSe₂ solar cell.

Figure 3-10 Variation in the short circuit current density in the absorber layer with the thickness of ZnO layer.
3.3.4 Thickness variation of the buffer (CdS) layer

The thickness of the buffer (CdS) layer was varied over the range 30 – 120 nm and its effect on the absorption of the absorber layer was studied. The thickness of the other layers is kept constant. The structural variation of thickness is shown in Table 3.7:

Table 3.7 CuInSe₂ solar cell structure with the thickness variation of buffer (CdS) layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>3.0×10⁶</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>4.0×10⁴</td>
</tr>
<tr>
<td>CIS</td>
<td>2.0×10³</td>
</tr>
<tr>
<td>CdS</td>
<td>30 – 120</td>
</tr>
<tr>
<td>ZnO</td>
<td>60</td>
</tr>
<tr>
<td>Al – Doped – Zno</td>
<td>75</td>
</tr>
</tbody>
</table>

The Q.E. of the active layer is compared with the Q.E. of the buffer layer in Figure 3-11 which allows tracking the effect of the thickness variation of the buffer layer on the Q.E. of the absorber layer.

The Q.E. of the two layers in Figure 3-11 is compared for the wavelength (λ) range 305 nm ≤ λ ≤ 1490 nm. The spectral range of Q.E. can be divided into different regimes; (a) 305 nm ≤ λ ≤ 500 nm, (b) 500 nm ≤ λ ≤ 1300 nm, (c) 1300 nm ≤ λ ≤ 1490 nm, (d) λ ≥ 1490 nm.

As seen in Figure 3-11 the low Q.E. of the active layer in the low wavelength range, 305 nm ≤ λ ≤ 500 nm, is a result of absorption in the buffer layer coupled with high absorption taking place in the ZnO:Al layer which gradually decreases while approaching the 500 nm mark. Consequently, an increase in the Q.E. of the active layer can be seen resulting in increasing absorption of high energy photons.
Figure 3-11 Comparison of the quantum efficiency of the ZnO layer (top) with the quantum efficiency of the absorber layer (bottom) with the variation in the thickness of the ZnO layer.

The Q.E. of the active layer keeps on increasing and reaches its maximum in the wavelength range, 500 nm ≤ λ ≤ 1300 nm. This is primarily due to the energy of the photons falling beyond/below the band gap energy of other layers. This high absorption is reflected in the low reflectance from the solar cell for the particular wavelength range.

There is a steep fall in the high wavelength range 1300 nm ≤ λ ≤ 1490 nm for the solar cell. This is due to rear surface passivation, increased absorption in the ZnO:Al as well the recombination taking place in the back contact layer. These photons fall beyond
the band gap energy of the TCO and buffer layer. This allows for the higher reflection of these photons from the solar cell.

The photons for wavelength $\lambda \geq 1490$ nm fall beyond the band gap of the TCO, buffer layer and active layer leading to their least absorption. They are reflected back into the atmosphere. The thickness dependence of the Q.E. of the active layer shows a trend of increasing with the decrease in the thickness of the buffer layer. The thickness reduction of the buffer layer has an effect on the Q.E. of the active layer.

Figure 3-12 Reflectance of solar cell with the variation in the thickness of the ZnO layer.

The dependence of the reflectance of the cell on the wavelength is shown in Figure 3-12. It is not affected by the variation in thickness of buffer layer in the wavelength range $305$ nm $\leq \lambda \leq 900$ nm. It shows a trend of increasing with the increase
in the thickness of the buffer for the higher wavelengths/lower energies. The thickness of buffer layer is reduced to 40nm so that it does not affect the absorption in active layer as well as there is reduced reflectance from the solar cell.

Figure 3-13 shows the dependence of the current and the reflection loss of the solar cell on the thickness of the buffer layer.

Figure 3-13 Variation in the short circuit current density in the absorber layer with the thickness of CdS layer.

The current in the active layer is found to decrease with the increase in the thickness of the buffer layer and the reflection loss increases, decreasing in the initial part and then increasing with the increase in the thickness of the buffer layer. The current and the loss do not increase/decrease in considerable amounts with minor changes in the
thickness of buffer layer beyond the point of 40nm. Thus, 40nm is the chosen thickness for the buffer layer of the CuInSe$_2$ solar cell.

### 3.3.5 Thickness variation of the back contact (Moly) layer

The thickness of the back contact layer was varied over the range 0.2µm – 1.0 µm and its effect on the absorption of the active layer was measured.

There was no change observed in the absorption of the active layer and reflection of the solar cell. This can be reasoned by the increased recombination in the back contact layer with increasing thickness of the same.

### 3.3.6 Optimum structure of the solar cell

The thicknesses of the various layers of the solar cell were varied and their effect on the performance of solar cell was studied. Different thicknesses of various layers of the solar cell were chosen to get the best performance from the solar cell. The optimal structure for the CIS solar cell with combination of ZnO and ZnO:Al as TCO of the solar cell was thus found to be:

Table 3.8 Structure of the CuInSe$_2$ solar cell with optimal thickness of each layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>$3.0 \times 10^6$</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>$4.0 \times 10^2$</td>
</tr>
<tr>
<td>CIS</td>
<td>$2.0 \times 10^3$</td>
</tr>
<tr>
<td>CdS</td>
<td>40</td>
</tr>
<tr>
<td>ZnO</td>
<td>60</td>
</tr>
<tr>
<td>Al – Doped – ZnO</td>
<td>75</td>
</tr>
</tbody>
</table>
Figure 3-14 and Figure 3-15 show the Q.E. of different layers of the solar cell as well as the overall reflectance of the cell for the wavelength range $305 \text{ nm} \leq \lambda \leq 1490 \text{ nm}$.

![Graph showing quantum efficiency of solar cell layers](image)

Figure 3-14 Quantum efficiency of all the layers of the optimal solar cell structure.

The values of current in the layers of the solar cell for the optimal structure are:
Table 3.9 Short circuit current density ($J_{sc}$) in the layers and reflection loss of the CuInSe$_2$ solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Current Density (mA/cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>0.00</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>0.52</td>
</tr>
<tr>
<td>CIS</td>
<td>42.62</td>
</tr>
<tr>
<td>CdS</td>
<td>1.78</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.19</td>
</tr>
<tr>
<td>Al – Doped – Zno</td>
<td>6.10</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>6.12</td>
</tr>
</tbody>
</table>

Figure 3-15 Reflectance of solar cell structure with optimum thickness of the layers.

3.4 Solar cell structure with TCO as a combination of ZnO and ITO
The structure of the solar cell is shown Table 3.10. The substrate is soda lime glass and other layers are then fabricated on top of it starting with molybdenum to indium-tin-oxide (ITO). The thickness of different layers of this solar cell structure was varied and their optimum values are calculated to generate the maximum current from the solar cell and reduce the reflection loss from the same. The structure with optimal thickness of each layer is shown in Table 3.10 along with the thickness.

Table 3.10 Optimal structure of CuInSe$_2$ solar cell with a combination of ZnO and indium-doped-tin oxide (ITO) as TCO.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>$3.0 \times 10^6$</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>$4.0 \times 10^2$</td>
</tr>
<tr>
<td>CIS</td>
<td>$1.8 \times 10^3$</td>
</tr>
<tr>
<td>CdS</td>
<td>50</td>
</tr>
<tr>
<td>ZnO</td>
<td>60</td>
</tr>
<tr>
<td>ITO</td>
<td>90</td>
</tr>
</tbody>
</table>

Figure 3-16 shows the comparison of the Q.E. of the different layers of the solar cell. The Q.E. is plotted for the wavelength range $305 \text{ nm} \leq \lambda \leq 1490 \text{ nm}$. This range is chosen since it spans the entire range of absorption of the active layer. Figure 3-16 can be subdivided into different spectral regions for analysis: (a) $305 \text{ nm} \leq \lambda \leq 600 \text{ nm}$, (b) $600 \text{ nm} \leq \lambda \leq 1300 \text{ nm}$, (c) $\lambda \geq 1300 \text{ nm}$. 
Figure 3-16 Quantum efficiency of the layers of the optimal structure of the solar cell.

The spectral region $305 \text{ nm} \leq \lambda \leq 600 \text{ nm}$ marks the low absorption by the absorber layer which increases to the maximum towards the end of this region. The low absorption in this region can be explained due high absorption in the TCO i.e. ZnO/ITO and buffer layer (CdS). The high energy photons are absorbed with more heat loss in this region.

In the spectral region $600 \text{ nm} \leq \lambda \leq 1300 \text{ nm}$; the absorber layer is at the highest of its absorbing capability. The TCO i.e. ZnO/ITO become optically transparent to the sunlight and allows the maximum of it to be passed to the absorber. The buffer layer shows no absorption and acts as a good transporter of the light. All of the photons in this range are absorbed by the solar cell providing a major contribution to the current produced by the same.
The Q.E. in the absorber layer starts declining for $\lambda \geq 1300$ nm and there is no absorption after $\lambda = 1490$nm. The photons beyond $\lambda = 1490$nm have energy less than the band-gap of the absorber layer due to which they are not absorbed by it. The absorbance in ITO and metallic back contact increases due to increased recombination in it and higher reflection which results in some absorption taking place in the ITO.

Figure 3-17 shows the dependence of the reflectance of the solar cell on the wavelength. The cell absorbs most of the incoming light and generates current till $\lambda = 1300$ nm. Below $\lambda = 1300$ nm there is high absorption in the absorber which does not allow for the photons to pass through. For $\lambda \geq 1300$ nm the absorption in all the layers of the solar cell is reduced leading to reflection of almost all of the photons back into the atmosphere. This region contributes more towards the reflection loss of the solar cell.

![Reflectance of the optimal solar cell structure](image.png)
The following values of current in the layers of the solar cell for the optimal structure are:

Table 3.11 Short circuit current density (J_{sc}) in the layers and reflection loss of the CuInSe₂ solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Current Density (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>0.00</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>0.58</td>
</tr>
<tr>
<td>CIS</td>
<td>45.17</td>
</tr>
<tr>
<td>CdS</td>
<td>2.48</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.19</td>
</tr>
<tr>
<td>ITO</td>
<td>3.01</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>5.90</td>
</tr>
</tbody>
</table>

The current in the different layers is calculated for the spectral range 305 nm ≤ λ ≤ 1490 nm to cover the whole absorption range of the solar cell. The lower absorption in the ITO layer allows for more photons to be absorbed in the absorber explaining the increased value of current compared to the solar cell structure with combination of ZnO/ZnO:Al as TCO. There is reduced reflection loss noted for this solar cell structure.

3.5 Solar cell structure with ITO as TCO

The structure of the solar cell under study is shown in Table 3.12. As in the previous sections, here also the thickness of the layers of the solar cell is varied generating the best thickness of each layer responsible for higher current generation and reduced losses in the solar cell. The optimal thicknesses of the different layers of the solar cell along with the respective layer name are shown in Table 3.12
Table 3.12 Optimum thickness of the layers of the CuInSe$_2$ solar cell structure with ITO as TCO.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>$3.0 \times 10^6$</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>$4.0 \times 10^2$</td>
</tr>
<tr>
<td>CIS</td>
<td>$1.8 \times 10^4$</td>
</tr>
<tr>
<td>CdS</td>
<td>40</td>
</tr>
<tr>
<td>ITO</td>
<td>105</td>
</tr>
</tbody>
</table>

The Q.E. of all the layers of the optimal structure of the solar cell is shown in Figure 3-18. The dependence of Q.E. on wavelength can be analyzed by subdividing the spectrum into the following regions: (a) $305 \text{ nm} \leq \lambda \leq 500 \text{ nm}$, (b) $500 \text{ nm} \leq \lambda \leq 1300 \text{ nm}$ and (c) $\lambda \geq 1300 \text{ nm}$.

The high absorption in the ITO in the spectral region $305 \text{ nm} \leq \lambda \leq 400 \text{ nm}$ results in reduced absorption in the absorber. The absorption in the absorber increases beyond $\lambda = 400 \text{ nm}$ but is still low due to absorption in the buffer (CdS) layer which reduces towards the end of this spectral range i.e. $400 \text{ nm} \leq \lambda \leq 500 \text{ nm}$.

The photons with energy in the range $500 \text{ nm} \leq \lambda \leq 1300 \text{ nm}$ are absorbed efficiently by the absorber layer due to reduced absorption in the other layers. The use of ITO as TCO does not become highly transparent and conductive towards the collection of electrons from the absorber layer resulting in less absorption in it as compared to the use of ZnO alone or ZnO in combination with ITO as TCO. There is not absorption in the buffer layer in this spectral range.

The wavelength region beyond $\lambda = 1300 \text{ nm}$ consists of the low energy photons which fall below the band-gap of the solar cell and are not absorbed by it. There in
absorption in the TCO i.e. ITO layer as well as recombination in the metallic back contact. There is least useful absorption in this range of wavelength.

Figure 3-18 Quantum efficiency of the layers of the optimal structure of the solar cell.
Figure 3-19 Reflectance of the optimal structure of the solar cell.

Figure 3-19 shows the dependence of the reflectance of the solar cell on the wavelength of light for the range $305 \, \text{nm} \leq \lambda \leq 1490 \, \text{nm}$. There is reduced reflection in the range $305 \, \text{nm} \leq \lambda \leq 1300 \, \text{nm}$. This can be attributed to improved absorption in the absorber layer and in some other layers of the solar cell. The recombination in the back contact allows for no addition to current but also no reflection loss from the solar cell. Beyond the wavelength $\lambda = 1300 \, \text{nm}$ the low-energy photons are not absorbed by the solar cell layers and are reflected back into the atmosphere.

The following values of current are calculated for the wavelength range $305 \, \text{nm} \leq \lambda \leq 1490 \, \text{nm}$ for the different layers of the structure with optimum thickness of the same:
Table 3.13 Short circuit current density ($J_{sc}$) in the layers and the reflection loss of the CuInSe$_2$ solar cell with ITO as TCO.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Current Density (mA/cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>0.00</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>0.53</td>
</tr>
<tr>
<td>CIS</td>
<td>45.80</td>
</tr>
<tr>
<td>CdS</td>
<td>2.18</td>
</tr>
<tr>
<td>ITO</td>
<td>3.37</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>5.45</td>
</tr>
</tbody>
</table>

The current generated by the solar cell is less due to absorption by the ITO used in combination with ZnO as TCO of the layer. The reflection loss is reduced compared to other structures. The lower resistivity of ITO does help in reducing the reflection loss of the solar cell compared to the other combinations of the TCOs for the solar cell.

3.6 Comparison

Table 3.14 shows the comparison of the different combinations of the TCO tested for the solar cell structure with Copper-Indium-Selenide (CIS) as the absorber layer.

1) Structure A is the CIS structure with combination of ZnO and Al-Doped-ZnO in the TCO layer

2) Structure B is the CIS structure with combination of ZnO and ITO in the TCO layer

3) Structure C is the CIS structure with ITO as TCO
Table 3.14 Comparison of the current generated and reflection loss of the solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Short Circuit Current Density in layers of the solar cell structure (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
</tr>
<tr>
<td>Absorber (CIS)</td>
<td>42.62</td>
</tr>
<tr>
<td>Buffer (CdS)</td>
<td>1.78</td>
</tr>
<tr>
<td>Back Contact (Moly)</td>
<td>0.52</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.19</td>
</tr>
<tr>
<td>Al-Doped-ZnO</td>
<td>6.10</td>
</tr>
<tr>
<td>ITO</td>
<td>-</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>6.12</td>
</tr>
</tbody>
</table>

The highest current and reduced reflection loss has been the major consideration in the choice of the optimum solar cell. The structure C using only ITO as the TCO for the solar cell is found to be satisfying the basic requirements of a good solar cell structure i.e. maximum short circuit current density and minimum reflection loss among all the other structures.

Thus, the best performing structure of the solar cell was found out by performing analytical calculations theoretically. There may be some practical issues which may not allow for the structure to perform as it should. The issues can vary from fabricating technologies, defects in the materials, environmental conditions and like.
Chapter 4

Copper-Indium-Gallium-Diselenide (CIGS) Solar cell

Copper-Indium-Gallium-Diselenide (CuInGaSe$_2$) has often been considered most promising for thin film solar cell fabrication. This is attributed partly to its low cost of fabrication and few microns thick high rate semiconductor deposition over large areas (Antonio Luque, 2003). The highest solar cell efficiency demonstrated with CuInGaSe$_2$ is 19.9% by NREL (Ingrid Repins, 2008). CuInGaSe$_2$ was the result of partial substitution of In with Ga in CuInSe$_2$ material. The band gap of the absorber layer in the CuInSe$_2$ solar cells could be increased from 1.02 eV to 1.2 eV by substituting In with Ga (Antonio Luque, 2003). The structure of a CuInGaSe$_2$ solar cell is shown in Figure 4-1:

Figure 4-1 Structure of the CIGS solar cell. (Manager, 2008)
The CuInGaSe$_2$ have shown long term stability in outdoor testing which makes them a promising material for the absorber layer in the solar cells. There are different methods available to fabricate the CuInGaSe$_2$ such as co-evaporation, two-step processing or selenization.

### 4.1 Material properties

CuInSe$_2$ can be alloyed in different proportions with CuGaSe$_2$ to yield CuInGaSe$_2$ with different band gaps. The possibility of alloying is attributed to the characteristics of CuInGaSe$_2$ to accommodate large variations in composition without appreciable difference in its optoelectronic properties (Antonio Luque, 2003).

The band gap (eV) for different compositions of CuInGaSe$_2$ can be calculated using the formula (M.I. Alonso, 2002):

$$E_g = 1.010 + 0.626x - 0.167x(1 - x)$$

Where

$$x = \frac{Ga}{Ga + In} = 0 - 1$$

The term 0.167 in the expression for band gap is known as the bowing coefficient. The dielectric constants of the CuInGaSe$_2$ used in this study are shown in the Figure 4-2. As seen from the curve the value of $\varepsilon_2$ goes to zero at 1.18 eV depicting that the band gap of the CuInGaSe$_2$ material used in the study is 1.18 eV.
The structure of the CIGS solar cell is used to evaluate the dependence of the optical parameters of a solar cell on the thickness of its constituent layers. The thickness of the different layers of the CIGS solar cell was varied and the thickness producing maximum current and reducing the reflectance of the cell were selected for the finding out the optimally thick structure of the solar cell. The general structure of the solar cell is shown in Table 4.1:

Table 4.1 General structure of the CIGS solar cell.

<table>
<thead>
<tr>
<th>Layer Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCO (Transparent Conductive Oxide)</td>
</tr>
<tr>
<td>CdS (Buffer Layer)</td>
</tr>
<tr>
<td>CIGS (Absorber or active layer)</td>
</tr>
<tr>
<td>Molybdenum (Back Contact)</td>
</tr>
<tr>
<td>Soda Lime Glass (Substrate)</td>
</tr>
</tbody>
</table>
The TCO layer of the above solar cell structure is used in the following combinations:

1) ZnO with Al-doped-ZnO

2) ZnO with Indium – doped – Tin Oxide (ITO)

3) Indium – doped – Tin – Oxide (ITO)

For each of the combination of TCO, the thickness dependence study of the optical properties of solar cell is carried out. This is performed in the following manner:

1) Thickness variation of Absorber Layer – The thickness of the absorber layer is varied and the thickness of the other layers is kept constant to get the optimum value of the absorber thickness which provides for increased current and reduced reflection loss.

2) Thickness Variation of the TCO – The TCO thickness is varied in the following way:
   a. If the TCO is a combination of two compounds then the thickness of each layer is varied and its effect on the optical properties of solar cell is observed and the best thickness is reported. For Eg: In a combination of ZnO and Al-doped-ZnO, the thickness of Al-doped-ZnO is varied initially and then, after selecting the best thickness of Al-Doped-ZnO the thickness of ZnO layer is varied to report the optimum value of the thickness of the layer.
   b. If TCO is only a single compound then the thickness of the layer is varied and the best thickness reported.
3) Thickness Variation of Buffer Layer – The thickness of the buffer layer (CdS) is varied and its effect on the absorbance, reflectance and transmittance of the solar cell is studied and the optimum thickness is then reported.

4) Thickness Variation of Back Contact – After having the optimum values of the thicknesses of the absorber layer, TCO’s and buffer layer; the dependence of the optical properties on the thickness of the back contact (Molybdenum) layer is studied.

The chapter is divided into the following subsections

1) Solar cell structure with TCO as a combination of ZnO and Al-doped-ZnO
   a. Structure of the solar cell with the optimal thickness of different layers

2) Solar cell structure with TCO as a combination of ZnO and ITO
   a. Structure of the solar cell with the optimal thickness of the layers of the solar cell.

3) Solar cell structure with TCO as ITO only
   a. Structure of the solar cell with the optimal thickness of the layers of the solar cell.

4) Comparison of the three best structures of CIGS solar cell

4.2 Solar cell structure with TCO as a combination of ZnO and Al–Doped–ZnO

The CIGS solar cell in the study uses TCO as a combination of ZnO and Al-doped ZnO (ZnO:Al). The thickness of different layers of the solar cell is varied and
optimum thickness of these layers has been calculated to provide for improved current and reduced losses. The structure is shown in Table 4.2:

Table 4.2 CIGS solar cell structure with ZnO and Al-doped-ZnO as TCO.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al – Doped – ZnO</td>
<td></td>
</tr>
<tr>
<td>ZnO</td>
<td></td>
</tr>
<tr>
<td>CdS</td>
<td></td>
</tr>
<tr>
<td>CIGS</td>
<td></td>
</tr>
<tr>
<td>Molybdenum</td>
<td></td>
</tr>
<tr>
<td>Soda lime glass</td>
<td></td>
</tr>
</tbody>
</table>

The structure of the solar with different layers and their respective thickness is shown in Table 4.3. The substrate model of the solar cell is used. Light falls on the TCO and passes through the absorber to the back contact and the either reflected or absorbed in the layers of the cell.

Table 4.3 CIGS solar cell structure with optimum thickness of each layer.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>3.0×10^6</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>4.0×10^2</td>
</tr>
<tr>
<td>CIGS</td>
<td>1.8×10^4</td>
</tr>
<tr>
<td>CdS</td>
<td>50</td>
</tr>
<tr>
<td>ZnO</td>
<td>90</td>
</tr>
<tr>
<td>Al – Doped – ZnO</td>
<td>70</td>
</tr>
</tbody>
</table>

Figure 4-3 shows the dependence of the Q.E. of the cell on wavelength. The wavelength spectrum used is 350 nm ≤ λ ≤ 1200 nm to cover the entire range for absorption by the absorber layer and to see the effect of the low energy photons on the
Q.E. of the cell. The spectrum can be subdivided into the sections: (a) 350 nm ≤ λ ≤ 500 nm, (b) 500 nm ≤ λ ≤ 1000 nm and (c) λ ≥ 1000 nm.

The absorbance of the TCO i.e. combination of ZnO/ZnO:Al and the buffer layer (CdS) is considerable for this spectral range. The Q.E. of the absorber layer increases with the decline in the absorbing power of the TCO and buffer layer. The Q.E. of the absorber progresses to the maximum towards the end of this region.

Figure 4-3 Quantum efficiency of the optimal structure of the solar cell with TCO as the combination of ZnO and ZnO:Al.

The photons are absorbed efficiently by the active layer in the spectral range 500 nm ≤ λ ≤ 1000 nm. The TCO/buffer layer do not interfere with the absorption. They behave as transparent to the passing photons allowing for high absorption in the active
layer. The presence of ZnO:Al reduces the absorption to some extent. The back contact recombination starts increasing towards the end of this region.

The Q.E. of the absorber falls as the energy of the photons falling on the cell reaches below the band-gap of the absorber for the spectrum $\lambda \geq 1000$ nm. The recombination in the back contact starts increasing along with absorption in the ZnO:Al layer. The lower energy photons tend to reflect back into the atmosphere from the solar cell.

![Figure 4-4 Reflectance of the optimal structure of the solar cell.](image)

Figure 4-4 shows the dependence of the reflectance of the solar cell on the wavelength spectrum $350$ nm $\leq \lambda \leq 1100$ nm. The reflectance is minimal for the wavelength spectral range $350$ nm $\leq \lambda \leq 1000$ nm due to high absorption in the other
layers of the cell. Beyond $\lambda = 1000$ nm the absorbing capacity of the cell is reduced. There is high recombination in the back contact and the rest of the photons are reflected back into the atmosphere. It is seen that there is high reflection from and recombination in the solar cell beyond the band-gap of the absorber layer.

The current in each of the layers of the optimal structure of the solar cell is shown in Table 4.4. The values show that the deposition of CIGS on molybdenum increases the collection of holes at the back contact. ZnO has negligible contribution to the current but the doping of ZnO with Al increases the absorption in the TCO. The current generated in the cell with TCO as the combination of ZnO and ZnO:Al is low due to high reflection loss and absorption in the other layers of the cell.

Table 4.4 Short circuit current density ($J_{sc}$) in the layers and reflection loss of the CIGS solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Current Density (mA/cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>0.00</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>3.17</td>
</tr>
<tr>
<td>CIGS</td>
<td>29.81</td>
</tr>
<tr>
<td>CdS</td>
<td>1.98</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.09</td>
</tr>
<tr>
<td>Al – Doped – Zno</td>
<td>4.71</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>7.09</td>
</tr>
</tbody>
</table>

The calculated values of the photocurrent generated by the analytical model were found to be lower by a ratio of 1.6 (Figure 4-5) compared to the experimental work (Olle Lundberg, 2003) performed on the CIGS absorber layer with same dielectric properties. This may be due to the superior quality of the film fabricated by the experimental group.
compared to the film used for modeling. Also, the other layers of the solar cell in the experimental setup would be fabricated in a different environment than the ones used in the simulation.

![Figure 4-5 Comparison of theoretical and experimental data. (Olle Lundberg, 2003)](image)

4.3 Solar cell structure with TCO as a combination of ZnO and ITO

The structure of the solar cell used in this section uses the combination of ZnO and ITO as the TCO of the solar cell. The light falls on the TCO and passes through the absorber to the back contact and then reflected back into the atmosphere. The structure of the cell along the thickness of the respective layers is mentioned in Table 4.5.
Table 4.5 Optimum thickness of the layers of the CIGS solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>$3.0 \times 10^6$</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>$4.0 \times 10^2$</td>
</tr>
<tr>
<td>CIGS</td>
<td>$1.8 \times 10^3$</td>
</tr>
<tr>
<td>CdS</td>
<td>50</td>
</tr>
<tr>
<td>ZnO</td>
<td>90</td>
</tr>
<tr>
<td>ITO</td>
<td>120</td>
</tr>
</tbody>
</table>

The thickness of the different layers of the solar cell is varied and best thicknesses of all the layers of the cell were calculated. Figure 4-6 shows the dependence of the absorbance of the different layers of the solar cell on the wavelength of the incident light. The incident light spectrum used here is $350 \text{ nm} \leq \lambda \leq 1200 \text{ nm}$. The spectrum can be subdivided into the following regions: (a) $350 \text{ nm} \leq \lambda \leq 550 \text{ nm}$, (b) $550 \text{ nm} \leq \lambda \leq 1000 \text{ nm}$ and (c) $\lambda \geq 1000 \text{ nm}$.

The Q.E. of the absorber layer is less in the initial portions of the region $350 \text{ nm} \leq \lambda \leq 550 \text{ nm}$. It increases to its maximum towards the end of the region. The absorption in the TCO and buffer layer is considerable in this region affecting the absorption in the absorber layer.

The absorption in the absorber is at its maximum in the wavelength region $550 \text{ nm} \leq \lambda \leq 1000 \text{ nm}$. The use of ITO with ZnO as TCO allows for higher absorption in the absorber by allowing more photons to pass through i.e. becoming optically transparent to the passage of the photons. The current generated by the cell is improved due to low resistivity of ITO compared to ZnO resulting in the combination of the two to be a good collector of the electrons.
Figure 4-6 Quantum efficiency of the optimal structure of the solar cell with TCO as the combination of ZnO and Indium-Tin-Oxide (ITO).

The absorption in the active layer of the cell reduces in the last spectral range due to increase in the absorption in ITO layer and recombination in the back contact. The high recombination towards the end of the spectrum and no absorption of the low energy photons increases the reflectance of the solar cell.
Figure 4-7 Reflectance of the optimal structure of the solar cell.

Figure 4-7 explains the dependence of the reflectance of the solar cell on the wavelength of the incident light. The reflectance is low in the spectral range $350 \text{ nm} \leq \lambda \leq 1000 \text{ nm}$ due to absorption in the other layers of the solar cell. The reflectance of the cell is lower compared to the structure of the cell using TCO as the combination of ZnO/ZnO:Al due to reduced absorption in the layers except the absorber and high collection of holes in the back contact for the low energy photons.

The current produced in the layers of the cell along with the respective layers is shown in Table 4.6. There is improvement in the current generated by the cell due to less absorption by the use of ITO along with ZnO. The reflection loss is also reduced due to
the fact that there is high collection of holes in the back contact. This structure proves to be better than the structure using TCO as the combination of ZnO/ZnO:Al.

Table 4.6 Short circuit current density (Jsc) in the layers and reflection loss of the CIGS solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Current Density (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>0.00</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>3.24</td>
</tr>
<tr>
<td>CIGS</td>
<td>32.51</td>
</tr>
<tr>
<td>CdS</td>
<td>2.14</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.07</td>
</tr>
<tr>
<td>ITO</td>
<td>2.53</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>6.34</td>
</tr>
</tbody>
</table>

4.4 Solar cell structure with ITO as TCO

The cell structure uses only ITO as the TCO of the solar cell. The thickness of the different layers of the cell is mentioned in Table 4.7 along with the layer names. The model of the cell is substrate here allowing the light to fall on the TCO and passing through the absorber to the back contact.

Table 4.7 Optimum thickness of the layers of the CIGS solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>$3.0 \times 10^6$</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>$4.0 \times 10^2$</td>
</tr>
<tr>
<td>CIGS</td>
<td>$1.8 \times 10^3$</td>
</tr>
<tr>
<td>CdS</td>
<td>50</td>
</tr>
<tr>
<td>ITO</td>
<td>120</td>
</tr>
</tbody>
</table>

Figure 4-8 shows the dependence of the Q.E. of the layers of the cell on the incident light spectrum. The structure used is the structure with optimal thickness and
best values for the generated current and reduced reflection and other losses. The spectrum consists of wavelength for the range $350 \text{ nm} \leq \lambda \leq 1100 \text{ nm}$.

Figure 4-8 Quantum efficiency of the solar cell structure with Indium – doped – Tin-Oxide (ITO) as TCO.

The Q.E. of the ITO and the buffer layer dominates the absorption in the wavelength range $350 \text{ nm} \leq \lambda \leq 450 \text{ nm}$. The Q.E. of the active layer increases towards its maximum in this range. The Q.E. of the TCO and buffer layer reduces for the remaining portion of the spectrum and the Q.E. of the absorber steadily increases to the maximum.

The absorption in the active layer is at its highest in the range $550 \text{ nm} \leq \lambda \leq 1000 \text{ nm}$. There is less absorption compared to the ideal absorption situation due to the fact that
some photons are also absorbed in the TCO i.e. ITO. The recombination in the back contact increases towards the end of this spectral range.

The remaining portion of the spectrum marks the sharp decrease in the Q.E. of the absorber layer due the lower energy of the photon and higher recombination in the back contact of the cell. The absorption in the ITO also increases towards the end of the spectrum still adding to the losses occurring in the cell.

Figure 4-9 shows the dependence of the reflectance of the cell on the wavelength. The reflection loss is lowered due to the recombination in the back contact and absorption in the TCO. The reflection loss is reduced due to the use of ITO as TCO.

Figure 4-9 Reflectance of the optimal structure of the solar cell.
The current generated by the cell is the maximum and appreciable depending on the current generated by other structures.

Table 4.8 Short circuit current density ($J_{sc}$) in the layers and reflection loss in the CIGS solar cell.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Current Density (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soda Lime Glass</td>
<td>0.00</td>
</tr>
<tr>
<td>Molybdenum</td>
<td>4.70</td>
</tr>
<tr>
<td>CIGS</td>
<td>32.71</td>
</tr>
<tr>
<td>CdS</td>
<td>2.30</td>
</tr>
<tr>
<td>ITO</td>
<td>3.11</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>7.08</td>
</tr>
</tbody>
</table>

The current generated in the different layers of the cell is mentioned in Table 4.8. There is high recombination in the back contact. The reflection loss is reduced compared to the usage of ZnO as TCO. There is contribution to the loss by absorption in the buffer and TCO layers.

4.5 Comparison

The comparison of the current generated and the losses in the different structures of the CIGS solar cell is mentioned in Table 4.9.

1) Structure A is the CIGS structure with combination of ZnO and Al-Doped-ZnO in the TCO layer

2) Structure B is the CIGS structure with combination of ZnO and ITO in the TCO layer

3) Structure C is the CIGS structure with ITO as TCO
Table 4.9 Comparison of the current generated and the reflection loss of the CIGS solar cell for different combinations of TCOs.

<table>
<thead>
<tr>
<th>Layer</th>
<th>Short Circuit Current Density in layers of the solar cell (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Absorber (CIGS)</td>
<td>A</td>
</tr>
<tr>
<td>Buffer (CdS)</td>
<td></td>
</tr>
<tr>
<td>Back Contact (Moly)</td>
<td>3.17</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.09</td>
</tr>
<tr>
<td>Al-Doped-ZnO</td>
<td>4.71</td>
</tr>
<tr>
<td>ITO</td>
<td>-</td>
</tr>
<tr>
<td>Reflection Loss</td>
<td>7.09</td>
</tr>
</tbody>
</table>

The structure using ITO as TCO generates the maximum short circuit current density. Using ZnO:Al in combination with ZnO increases the losses due to higher absorption in it. The structure using ITO as TCO is chosen to be the optimal structure due to higher current generated which forms the major consideration in the choice of optimum structure of the cell.

There may be some practical restrictions in the fabrication of the cell due to environmental degradation, performance of the material over time, defects and others which are out of scope of the work of this thesis.
Chapter 5

Conclusions and future work

This thesis addressed a methodology allowing for the test and optimization of different materials which can be used in the solar cells. These materials can be used for the purpose of being used as transparent conductive oxides (TCOs), buffer layers, back contacts, substrates and the absorber layers. The materials can range from anything to anything. All we need for the test are the dielectric constants of the materials used in the structure of the cell, at different wavelengths of the spectrum. The tool calculates the quantum efficiency of different layers of the cell, the reflectance and the transmittance of the cell. The results of the tool eventually allow for the choice of the materials constituting high efficiency solar cells.

There is the factor of cost-effective manufacturing and distribution related to a business. The thinning of different layers of the solar cell is important to find out if there is a possibility to achieve higher efficiency by reducing the thickness of the layers. The methodology also allows for the optimization of the thickness of the different layers of the solar cell which eventually helps to improve the cost-effectiveness of the manufacturing process.
5.1 Conclusion

The work presented in this thesis allows for the calculation of the current generated by the solar cell by incorporating the physics behind the optical modeling with the different layers of the solar cells. We try to find out different methods to improve the absorption and reduce the reflection and transmission from the solar cell.

Chapter 3 uses a CuInSe₂ solar cell and applies the thickness optimization technique to it. The thickness of the layers of the solar cell has been varied to ascertain the optimal thicknesses of the same. The different combinations of TCOs allowed the analysis of the effect of the TCO material on the performance of the solar cell. The reduction in thickness of the layers and the choice of TCO material help us to provide for better absorption and reduced reflectance and transmittance. The cell structure Soda-lime-glass/Molybdenum/CuInSe₂/ITO was chosen to be the most efficient with a short-circuit current density of 45.80 mA/cm² and a reflection loss of 5.45 mA/cm².

In Chapter 4 the thickness optimization and TCO material variation was applied to the CIGS solar cell structure mentioned in Chapter 4. The solar cell structure Soda-lime-glass/Molybdenum/Cu(In,Ga)Se₂/ITO was chosen to be the optimal cell. The choice was based on the high short circuit current density. The short circuit current density for the cell structure was 32.71 mA/cm² and the reflection loss was 7.08 mA/cm².

5.2 Future work

The tool considers the layers of the solar cell to be a mechanical stack of materials of some thickness. The layers are flat and smooth allowing the light to be incident, reflected and transmitted. There is no scattering involved in the travel of light. Scattering
occurs when there interface between two layers of the cell are not flat and smooth but rather they are rough and intermingled with each other due to some reaction between the materials. Due to roughness at the interface the light scatters in different directions which cannot be calculated by applying the basic principles of the reflection and refraction. The principles have to be modified to incorporate the effect of scattering in the solar cells.

The incident light in this tool is considered to be un-polarized. This is true for sunlight. Polarization can be included in the physics used in this tool to expand its usage from analytical modeling for solar cells only to being used in spectroscopic ellipsometry which is important for detection of accurate material properties.
References


   http://pvedrom.pveducation.org/CELLOPER/QUANTUM.HTM


