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Modeling, Simulation and Characterization of Optoelectronic Properties of 2D-3D CoO-ATO Nano Structures

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Modeling, Simulation and Characterization of Optoelectronic Properties of 2D-3D CoO-ATO Nano Structures

by

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of the requirements for the degree of
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DEDICATION

To Dad and Mom who always cherished my inquisitive attitude and to Professor Sylvia W Thomas

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TABLE OF CONTENTS

LIST OF TABLES		iii
LIST OF FIGURES		iv
ABSTRACT		vi
CHAPTER 1	INTRODUCTION	1
1.1	Structure of Thesis	1
1.2	Background and Motivation	2
1.3	Current State of Art	3
1.4	Hypothesis and Research Objectives	6
CHAPTER 2	MATERIAL FUNDAMENTALS	7
2.1	Electro-Magnetic in Metals and on Metal Surfaces	7
2.2	The AM1.5g Solar Spectrum	8
2.3	Ultimate Efficiency	9
2.4	Overview of Light Trapping Effect	9
CHAPTER 3	OVERVIEW OF COBALT OXIDE ANTIMONY DOPED TIN OXIDE NANOSTRUCTURES	10
3.1	Optical Property of Cobalt Oxide (CoO)	10
3.2	Optical Property of Antimony Doped Tin Oxide (ATO)	10
3.3	Polystyrene	11
3.4	Toluene	12
3.5	Preparation of the Solution	12
CHAPTER 4	MORPHOLOGICAL AND OPTICAL CHARACTERIZATION OF 2D-3D COBALT OXIDE ANTIMONY DOPED TIN OXIDE STRUCTURE	14
4.1	Wafer Cleaning	14
	4.1.1 RCA Cleaning	14
	4.1.2 Acetone-Methanol Cleaning	15
4.2	Spin-Coating	17
4.3	Scanning Electron Microscopy (SEM)	18
4.4	Ellipsometry	20
4.5	Refractive Index Measurement of CoO-ATO	20
CHAPTER 5	MODELING AND SIMULATION OF OPTOELECTRONIC DEVICE	23
5.1	Proposed Model	23

5.2	Construction of Silicon Substrate	23
5.3	Modeling of Optoelectronic Device with Thin Film Antireflective Coating	24
CHAPTER 6	COMPARATIVE ANALYSIS OF THE ABSORPTION EFFICIENCY OF OPTOELECTRONIC DEVICE WITH THIN FILM AND NANO FIBER MEMBRANE ANTI-REFLECTIVE COATING	26
CHAPTER 7	CONCLUSION AND FUTURE WORK	31
7.1	Future Work	32
REFERENCES		33
APPENDIX A: CST WORKING MODULE		35
APPENDIX B: GLOSSARY OF TERMS		36
APPENDIX C: SOFTWARE		37
ABOUT THE AUTHOR		END PAGE

LIST OF TABLES

Table 1.1	Absorption efficiency of silicon solar cell with embedded silver nano sphere of different diameters	5
Table 1.2	Absorption efficiency of silicon solar cell with embedded aluminum nano sphere of different diameters	5
Table 3.1	Chemical composition by weight of CoO-ATO solution used in the thesis	12
Table 3.2	Chemical composition by volume and mass used for making solution used in the thesis	13
Table 4.1	Refractive index of CoO-ATO across the visible spectrum	21
Table 5.1	Material parameter of the silicon substrate used as reference	24
Table 6.1	Summary of absorption efficiency	29

LIST OF FIGURES

Figure 1.1	Metal nano sphere	4
Figure 1.2	Design of the thin film plasmonic solar cell	5
Figure 2.1	AM1.5g solar spectrum	8
Figure 3.1	Structure of polystyrene	11
Figure 3.2	Chemical structure of toluene	12
Figure 4.1	RCA wet bench, NREC, University of South Florida	15
Figure 4.2	Chemicals for Acetone-Methanol cleaning, in fumehood, Surface Science Laboratory, University of South Florida	15
Figure 4.3	Substrate transferred from Acetone to Methanol in fumehood, Surface Science Laboratory, University of South Florida	16
Figure 4.4	Cleaned substrate, securely stored	16
Figure 4.5	Speedline technology spincoater, Model P6700 Series, NREC, University of South Florida	17
Figure 4.6	Polished silicon substrate spin coated with CoO-ATO Solution, NREC, University of South Florida	18
Figure 4.7	Scanning electron microscopy of CoO-ATO nanofiber formed from 0.2% Cobalt Oxide by weight	19
Figure 4.8	Refractive index of CoO-ATO over visible spectrum	22
Figure 4.9	Extinction coefficient of CoO-ATO over visible spectrum	22
Figure 5.1	Silicon substrate	23
Figure 5.2	Unit cell of thin film antireflective coating over the reference model	24

Figure 5.3	Unit cell of nanofiber membrane antireflective coating over the reference model	25
Figure 5.4	Electric dispersion of CoO-ATO	25
Figure 6.1	Thin film silicon solar cell	26
Figure 6.2	Transmission coefficient, reflection coefficient and absorption of CoO-ATO thin film	28
Figure 6.3	Transmission coefficient, reflection coefficient and absorption of CoO-ATO nanofiber membrane	29
Figure 6.4	Absorption efficiency of optoelectronic device with no antireflective coating (Silicon), and optoelectronic device having antireflective coating in the form of thin film and nanofiber membrane of CoO-ATO	30
Figure A.1	CST Microwave Studio Suite (Design window)	35
Figure A.2	CST Microwave Studio Suite (S-parameter window)	35

ABSTRACT

Devices for converting solar energy to electrical energy are not considerably efficient, though there are abundant renewable solar energy sources. Therefore there is a continuous call for investigation of new devices that are efficient and eco-friendly thereby contributing to harvested energy technology.

This thesis characterizes the optical constant (refractive index) of a novel material, cobalt oxide-antimony doped tin oxide (CoO-ATO). Thin film of CoO-ATO is generated using spin coating of CoO-ATO solution having 76.33% chloroform, 13.47% polystyrene, 10% antimony doped tin oxide and 0.2% cobalt oxide by weight. The thin film is analyzed through ellipsometry to acquire the refractive index of the material through the visible spectrum, which is used for modeling an antireflective coating in a solar cell. The model is designed and analyzed by simulation using computer simulated technology, and the results of the analysis of a thin film or a nanofiber membrane of the novel material implemented as an antireflective coating layer that affects the absorption efficiency of the optoelectronic device.

The result of the analysis showed enhancement of absorption efficiency within the visible spectrum for both thin film and nanofiber membrane of the novel material CoO-ATO. The absorption through thin film was more than that of the nanofiber membrane.

CHAPTER 1: INTRODUCTION

1.1. Structure of Thesis

Introduction of the thesis explains the significance of the novel material, Cobalt Oxide Antimony doped Tin Oxide (CoO-ATO), chosen for the research, its characterization and implementation of its 2D-3D form in optoelectronic devices, for analysis and understanding if introducing a layer of the material as an antireflective coating to affect absorption efficiency of the device.

A primary interest of the research is investigating the CoO-ATO nano structures to be used in solar cell for enhanced absorption thereby increasing the cell efficiency. In this thesis the optical properties of CoO-ATO are characterized and are used for modeling and simulating in computer simulated technology (CST) to analyze the absorption pattern of the material and hence absorption efficiency of the optoelectronic device.

The second chapter presents the fundamental properties, mathematics and physics that are applied to the material, used for characterizing and modeling the material.

In the third chapter the overview of CoO-ATO nano structures are presented. The properties of both CoO and ATO are elaborately discussed and classification of the nano structures as thin film and nanofiber membrane along with their preparation under laboratory conditions are discussed.

Morphological and optical characterization is discussed in detail in chapter four. This chapter discusses the spin coating, scanning electron microscopy (SEM), ellipsometry used for material characterization and measurement of refractive index of CoO-ATO.

Chapter five presents the simulation of silicon substrate and the optoelectronic device with antireflective coating. In this chapter the S-Parameters that are obtained from the simulated results are presented. The overall absorption profile and absorption efficiency of the silicon substrate and the optoelectronic device is also presented in this chapter.

Chapter six will present the summary of the findings of the research and discusses the future work.

1.2. Background and Motivation

Growing energy requirement worldwide is primarily covered by fossil fuel. Exhaustion of fossil fuel places the matter into concern, as damaging of eco system and global heating are some undesirable effects. This brings about a thought of designing and developing an eco-friendly energy harvesting device. The term photovoltaic refers to a process which makes a direct conversion of solar energy to electrical energy.

Developing efficient photovoltaic devices is one of the solutions of reducing the larger dependency on fossil fuels and environmental hazards caused from the exhaustion of fossil fuels. Such a device also enables us using solar energy, which can be considered to be the most abundant form of renewable energy reaching the earth, promoting green energy and reducing negative environmental impact. Adoptions of such photovoltaic devices are increasing due to increased production and lower price of the device. However, low cost and higher efficiency photovoltaic devices are required for renewable energy such as solar energy to contribute as a substantial energy resource.

For enhancing the efficiency and reducing the cost of the harvested energy scientists are looking forward to novel materials that could be implemented in the device to produce energy efficient optoelectronic devices. This thesis considers a novel material, CoO-ATO, which could be implemented as a layer in the optoelectronic device to enhance the absorption within the visible spectrum. The research outlines a procedure of characterizing the optical properties of CoO-ATO and uses the properties to model and simulate optoelectronic device for harvesting green energy.

Cobalt oxide antimony doped tin oxide (CoO-ATO) is the choice of material as the novel material proven to be a promising material having thermal reflective property. Findings of the previous research states increased surface area increases the infrared reflectivity and hence the thesis introduces a nanofiber membrane of the novel material which increases the surface area significantly making it a better anti reflective coating.

1.3. Current State of Art

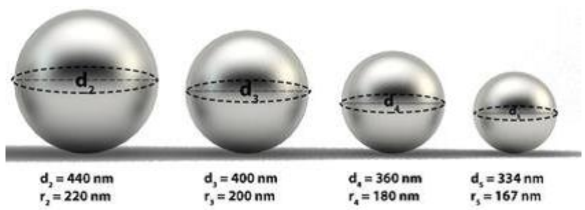
Recently, solar cells incorporating plasmonic structures are well-thought-out to be a promising device capable of attaining high absorption and overall efficiency. [2][14]

Thin film Silicon (Si) solar cell's absorption efficiency can be improved by introducing metal nano particles into the cell structure adjacent to surface of the silicon substrate as a top layer. Versatile optical engineered tool like metal nano particle (plasmonic structures) has the potential to enhance device efficiency and reduce the cost of harvesting most abundant form of renewable energy the solar energy. [14]

Modeling of arrayed silver and aluminum nanoparticle individually over a 3μm thin film Silicon substrate yielded improved optical absorption over the visible spectrum. The model that has been developed with different radius of silver (Ag) and aluminum (Al) nano sphere located adjacent to the Si substrate. The radius of the nano-sphere were changed each time before simulation. Changing radius showed difference in absorption profile and absorption efficiency of the optoelectronic device. [14]

Ridita et. al said surface Plasmon resonance effect is displayed by silver nano particle and plasmon excitation efficiency [4][14]. However, nano particle like aluminum compared to silver shows optical resonance across a much broader region of the visible spectrum [5][14].

Silver and aluminum nano particle of different radius are distinctively introduced adjacent to silicon substrate.



(a) Metal nano sphere of different radius

(b) Close packed metal nano sphere on top of silicon thin film

Figure 1.1: Metal nano sphere

The design of the model is done using computer simulated technology and the transmission and reflection coefficient are recorded. Absorption coefficient is obtained using the energy balance equation. The final design of the model is given below.

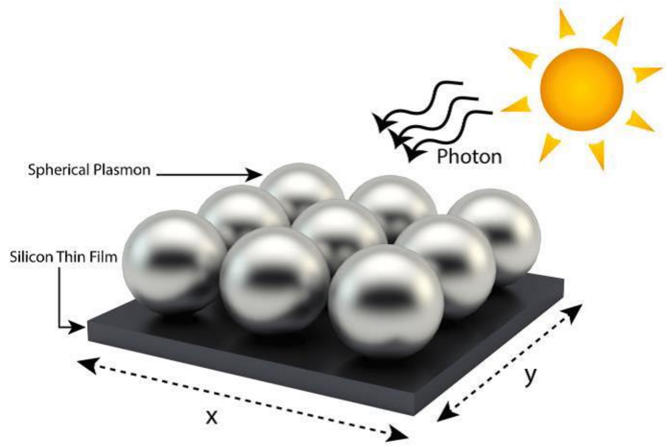


Figure 1.2: Design of the thin film plasmonic solar cell

The absorption efficiency of the optoelectronic device is quantified using ultimate efficiency equation with embedded nano particles. The efficiencies are presented in table below.

Table 1.1: Absorption efficiency of silicon solar cell with embedded silver nano sphere of different diameters

Diameter of Ag nano sphere (nm)	167	180	200	220
Absorption Efficiency (%)	19.47	20.09	22.48	21.62

Table 1.2: Absorption efficiency of silicon solar cell with embedded aluminum nano sphere of different diameters

Diameter of Al nano sphere (nm)	167	180	200	220
Absorption Efficiency (%)	21.47	22.15	24.06	23.58

Results of current state of art affirmed embodiment of metal nano particle enhances the absorption in optoelectronic device across visible spectrum.

Electrical response of silicon solar cell with a thin film of CoO-ATO coating is also recorded. Solution (polymeric in nature) of cobalt oxide-antimony doped tin oxide (CoO-ATO) used for spin coating thin film over 3" x 6" Si solar cells.[15] Improved response of the solar cell is hypostatized by considering the spectral response of the material. Obtained results gave maximum wattage at 16% cobalt by weight and 94% antimony by weight.[14]

1.4. Hypothesis and Research Objectives

In this thesi the optical constant (refracting index) of CoO-ATO thin film will be characterized using ellipsometry. Optical resonance of CoO-ATO across a broader region (visible spectrum) is used to modeling a solar cell with higher absorption efficiency.

It is hypothesized that spin coating produce a thin film can be used to analyze and measure refractive index of CoO-ATO which can be used for modeling and simulating the layer of the material into the optoelectronic device.

The research objectives are as follows

1. Fabricate a thin film of CoO-ATO and characterize the optical property of CoO-ATO.
2. Model and simulate solar cell with 2D/3D nanostructure of CoO-ATO and analyze the absorption pattern to work out the absorption efficiency of the optoelectronic device with a layer of antireflective coating of the novel material.

CHAPTER 2: MATERIAL FUNDAMENTALS

2.1. Electro-Magnetic in Metals and on Metal Surfaces

Characterization of the optical property of 2D-3D nanostructure and modeling are required to be analyzed and quantified using mathematics which will be provided in this chapter. Also the basic properties and characteristic of materials will be reviewed.

When electro-magnetic field interacts with the surface of the metal the following mathematical Maxwell equations applies:

$$\nabla . D = \rho \quad 2.1$$

$$\nabla . B = 0 \quad 2.2$$

$$\nabla \times D = -\frac{\delta B}{\delta t} \quad 2.3$$

$$\nabla \times H = J + \frac{\delta D}{\delta t} \quad 2.4$$

Here E is the dielectric field, D is the dielectric displacement, H is the magnetic field and B is the magnetic induction. Also the charge density (external) is defined with the parameter ρ and current density is defined with the parameter J.

For non-magnetic, linear and isotropic media, the dielectric displacement and the magnetic induction is defined as:

$$D = \epsilon_0 \epsilon E \quad 2.5$$

$$B = \mu_0 H \quad 2.6$$

$\epsilon = \epsilon(\omega)$ the dielectric constant which is frequency dependent and can be presented as a complex function in general, $\epsilon = \epsilon' + i\epsilon''$. It can be associated with the complex index of refraction as $n = n + ik = \sqrt{\epsilon}$. From the above consideration the following is obtained:

$$\epsilon' = n^2 - k^2 \tag{2.7}$$

$$\epsilon'' = 2nk \tag{2.8}$$

$$n^2 = \frac{\epsilon\prime}{2} + \frac{1}{2}\sqrt{(\epsilon'^2 + \epsilon''^2)} \tag{2.9}$$

The refractive index n (real part) is accountable for the dispersion within the medium; the imaginary part $k(\omega)$ (extinction coefficient) governs the absorption. [1]

2.2. The AM1.5g Solar Spectrum

The AM1.5g solar spectrum G_λ the AM1.5g absorption factor A is obtained

$$A = \frac{\int A_\lambda G_\lambda \, d\lambda}{\int G_\lambda d\lambda} \tag{2.10}$$

This AM1.5g spectrum is a standardized solar spectrum given by Hulstrom and is shown in figure 2.1.

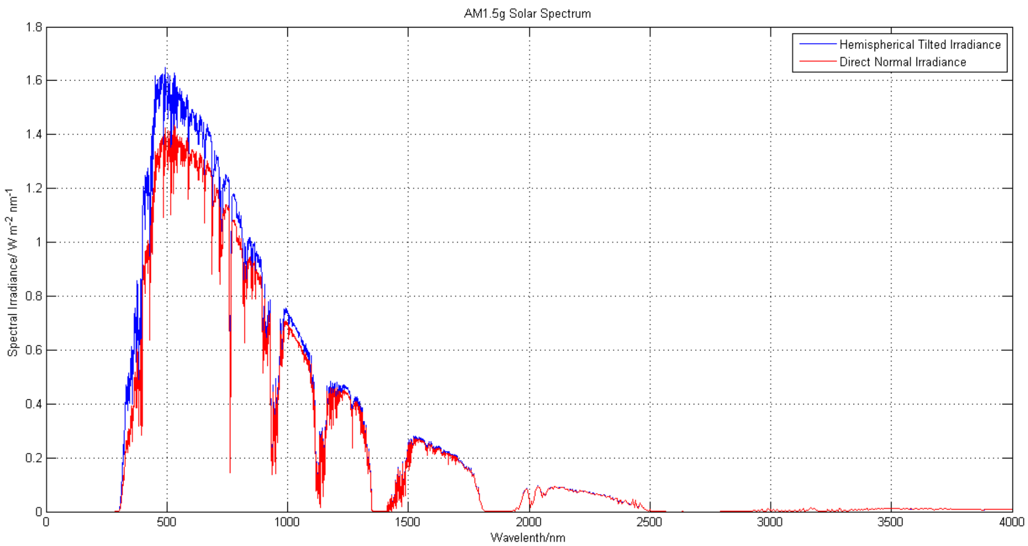


Figure 2.1: AM1.5g solar spectrum

AM1.5 refers the Air Mass 1.5 and 'g' is the global spectrums that has both diffused and direct solar irradiance. Similarly, a spectral reflection factor R_λ and spectral transmission factor T_λ can be defined for the laminate, from which the corresponding AM1.5g reflection factor R and AM1.5g transmission factor T can be derived. From conservation of energy it follows. [2]

$$R_\lambda + T_\lambda + G_\lambda = 1 \quad 2.11$$

2.3. Ultimate Efficiency

The absorption efficiency enhancement is quantified using the ultimate efficiency [15] defined as

$$\eta = \frac{\int_{800nm}^{\lambda g} A(\lambda)\, I(\lambda) \frac{\lambda}{\lambda g}\, d\lambda}{\int_{800nm}^{4000nm} I(\lambda)\, d\lambda} \quad 2.12$$

where, bandgap of silicon is represented by the wavelength λ_g and λ is the wavelength. $I(\lambda)$ is the AM1.5 Solar spectral irradiance [3], $A(\lambda)$ refers to the overall absorbance of metal nano particle or thin film or nanofiber membrane .

2.4. Overview of Light Trapping Effect

Si as an indirect band gap material has the nature of limited absorption when the thickness is very thin. This limited absorption reduces the efficiency of the optoelectronic device. To improve efficiency of the thin film Si solar cell, Light trapping mechanism is used by increasing the OPL and to prevent light that otherwise would be lost [5].

OPL is the total distance of light travels in the thin film silicon solar cell. Light trapping technology is able to diffract and reflect light inside the cell, such that that light bounces back and forth inside the cell, results in increases of OPL [5].

CHAPTER 3: OVERVIEW OF COBALT OXIDE ANTIMONY DOPED TIN OXIDE NANOSTRUCTURES

Detail of chemical structures and optical property of CoO and ATO will be discussed individually in this chapter. Detail of preparation of CoO-ATO solution will be given which yield uniform thin film over polished silicon and glass substrate. Preparation of Nano fibers will be discussed and dimension of CoO-ATO nanoparticle will be given.

3.1. Optical Property of Cobalt Oxide (CoO)

Cobalt oxide, a transition metal oxide is promising for application in the field of science. The CoO oxide used in this thesis is a stable oxide.

This thesis characterizes the optical property of the novel material, CoO-ATO. The characterization required analysis of the optical property of cobalt oxide. Spectroscopic ellipsometry (SE) is an appropriate, precise and surface-sensitive techniques to examine the complex index of refraction, $N = n - ik$ (optical constant) and the thickness of the film.[6]

The refractive indices obtained are similar to those described in the literature for CoO (2.4 plus minus 0.2).[7][8][9][10] Differences in the index of refraction for CoO informed in the literature are due to the method of preparation of the films.[11]

3.2. Optical Property of Antimony Doped Tin Oxide (ATO)

High electrical conduction, optical transmission and infrared reflection make doped tin oxide a potential candidate for optoelectronic device.

Numerous techniques can be applied to prepare films of tin oxide such as chemical vapor deposition, spray pyrolysis, reactive rf sputtering, vacuum evaporation etc. [12]. However, films obtained from spray technique yield high optical transmission and low sheet resistance [12]. Shanti et. al. reports transmission of wavelength in the range 0.33 to 2.0µm and reflection within 0.33 to 10.0µm in both undoped and doped tin oxide [14]. Plasma resonance occurring at 3.2µm due to the reflection in undoped tin oxide film is also reported. The film is highly trans-missive over 0.4 to 2.0µm [14]. The pattern of transmission is different in doped tin oxide film. It is reported that transmission increases 1.4-m/o Sb concentration and decreases if antimony is added and in case of doped antimony near infrared region plasma resonance occurs because of high concentration of free carriers 10^{20} /cm^3 [14]. In infrared region reflection increases with increased concentration of Sb up to 3-m/o as mobility and carrier concentration are factors on which reflection depends upon. Reflection decreases when doped at the range of 10-m/o due to low mobility [14]. Since the carrier concentration in the film is 10^{20} /cm^3, the optical phenomenon in the near infrared region is described by the Drude theory [14].

3.3. Polystyrene

Polystyrene is an atomic polymer can be made from styrene monomer. Chemical structure of polystyrene is given in figure 3.1.

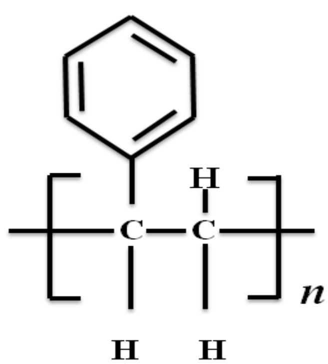


Figure 3.1: Structure of polystyrene

Polystyrene is inexpensive and general purpose one is clear (naturally transparent). It is used as the base material for ATO and CoO because of its wide availability and safe handling property. As the figure shows the chemical structure is composed of long chain of hydrocarbon where alternate carbon atom is bonded with a phenyl group (benzene). it is chemically inert and non biodegradable. It is insoluble in water but highly soluble in acetone. It has a refractive index of 1.6 [16].

3.4. Toluene

Structure of toluene is given in Figure 3.2. It is a colorless liquid and can be used as solvent. At 20ºC it has a refractive index of 1.497 [17].

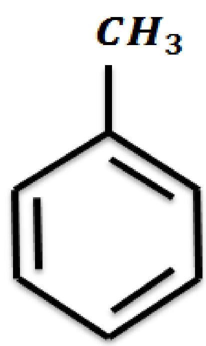


Figure 3.2: Chemical structure of toluene

The sample we used for fabricating thin films have ATO (solgel) nanoparticles dispersed in toluene.

3.5. Preparation of the Solution

The solution used for making thin film and the nano fiber membrane of CoO-ATO has the following composition by weight.

Table 3.1: Chemical composition by weight of CoO-ATO solution used in the thesis

Chemicals	**Percentage (%) by weight**
Chloroform	76.33
Polystyrene	13.47
Antimony doped tin Oxide (ATO)	10
Cobalt Oxide (CoO)	0.2

Chemical composition by volume and mass of the chemical used for generating the thin film and nano fiber membrane are as follows:

Table 3.2: Chemical composition by volume and mass used for making solution used in the thesis

Chemicals	**Percentage by volume/ml and mass/g**
Chloroform	3ml
Polystyrene	0.782894g
Antimony doped tin Oxide (ATO)	0.670373ml
Cobalt Oxide (CoO)	0.011624g

CHAPTER 4: MORPHOLOGICAL AND OPTICAL CHARACTERIZATION OF 2D-3D COBALT OXIDE ANTIMONY DOPED TIN OXIDE STRUCTURE

Scanning electron microscopy, spin coating and ellipsometry will be discussed in detail in this chapter which assisted in material characterization.

4.1. Wafer Cleaning

Cleaning the substrate is a primary step before beginning the experimental procedure. The substrate can be clean using standard steps before processing begins in the experiment.

4.1.1. RCA Cleaning

RCA (Radio Corporation of America) clean removes organic residue, ion contamination and oxide layers.

Solutions applied in the cleaning procedure are “RCA standard clean” commonly known as SC-1 and SC-2. The RCA SC-1 contains aqueous hydrogen peroxide, aqueous ammonium hydroxide and deionized water in the ratio of 1:1:5. SC-2 contains aqueous hydrochloric acid, hydrogen peroxide and deionized water in the ratio of 1:1:6.

SC-1 dissolves organic substance and removes impurities (particles). If there are and trace of ionic contamination then SC-2 will completely remove it preventing further contamination.

Figure 4.1: RCA wet bench, NREC, University of South Florida

4.1.2. Acetone-Methanol Cleaning

The substrate can also be cleaned using acetone, methanol and DI water. The procedure can be used to remove residues, debris and photoresists from the substrate. The cleaning process is carried out generally in fumehood. Glass beakers, tweezer, nitrogengun and texwipes are required.

Figure 4.2: Chemicals for Acetone-Methanol cleaning, in fumehood, Surface Science Laboratory, University of South Florida

For our substrate cleaning two 150ml glass beaker is taken, one partially filled with acetone and the other partially filled with methanol. The wafer is first submerged in the beaker containing acetone for 10 minute and transferred carefully to the beaker containing methanol using tweezer and submerged for next 10 minute.

Figure 4.3: Substrate transferred from Acetone to Methanol in fumehood, Surface Science Laboratory, University of South Florida

These chemicals removes the debris and residues in the substrate. The substrate is carefully removed from methanol and washed with DI water and dried using nitrodgen gun before storing it securely.

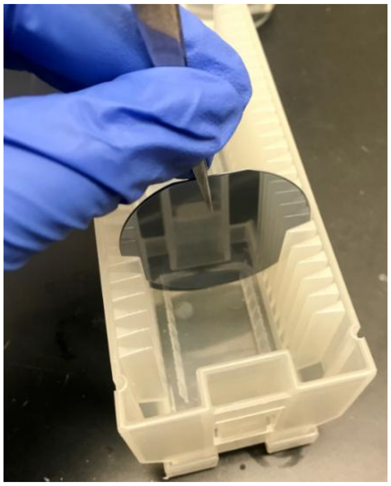


Figure 4.4: Cleaned substrate, securely stored

This thesis uses RCA or Acetone-Methanol cleaning to clean the substrate before spin coating a thin film of the novel material, CoO-ATO. After Spin coating ellipsometry is performed over the visible spectrum to characterize the optical property of the material.

4.2. Spin-Coating

Deposition of thin film over a substrate can be done spin coating. In the technique the substrate is held in the machine using a vacuum suction. To maintain the grip the vacuum pump is turned on throughout the course. The substrate is then covered with the coating material. Once the spin coater turns on the substrate rotates at adjusted speed to form a coating of thin film over the substrate. The centrifugal force is responsible for spreading the material and forming a uniform thin film.

Figure 4.5: Speedline technology spincoater, Model P6700 Series, NREC, University of South Florida

Thin film used in this thesis was made of a liquid solution of the novel material, CoO-ATO, spin coated over a polished silicon substrate. The viscosity of the solution and the speed and time of rotation were the parameters that were controlled to have uniform thin film using Speedline Technology Spincoater at NREC, University of South Florida.

Total ramp time for the spin coating is 234s. As the machine starts to operate in first five second it will reach 4000rpm and in next five second it will reach 6000 rpm.

Figure 4.6: Polished silicon substrate spin coated with CoO-ATO Solution, NREC, University of South Florida

4.3. Scanning Electron Microscopy (SEM)

Initial idea of scanning of Scanning Electron Microscopy (SEM) is to expose a sample to a fine collimated beam of X-ray (or other chosen beam) by a transverse movement of the sample towards beam. Then a receptive recording device measures the degree of interaction between the sample and the beam. The recorded sample is then amplified and the amplified sample is demonstrated on an electron tube. The main idea of the procedure is to determine the accurate dimension of a nano scaled particle which cannot be analyzed with light microscopy. [18]

One of the major parts of the conventional SEM machine is the microscope column consisting an electron gun, a pair (or one) condenser lenses, beam deflection coil, some apertures and an objective lens. The specimen chamber is located at the lower end of the microscope column. The chamber has a detector and a specimen stage. The detector detects different signals produced by the interaction of the electrons and specimens. High vacuum pump together with pre vacuum evacuates both microscope column and specimen chamber. A pressure of about 10^{-4} Pa is maintained in the specimen chamber. This allows the electron beam to travel to the specimen without deviation. [18]

The other major part of the machine is the electronics console which accelerates the voltage with its electric supply. It also has components like scan generator, objective lenses, condenser and electronic amplifier for amplification of the obtained signal. This part also has monitors connected to it that displays the image and micrographs. [18]

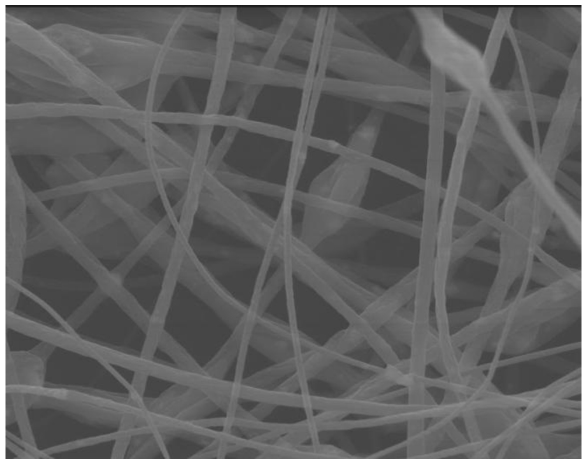


Figure 4.7: Scanning electron microscopy of CoO-ATO nanofiber formed from 0.2% Cobalt Oxide by weight

In this thesis the Hitachi field emission scanning electron microscope (FE-SEM), in nanotechnology research and education center (NREC) at University of South Florida, was used for the analysis of the cobalt oxide nano particle. The diameter of the particle was obtained from SEM. A solar cell is model having cobalt oxide nano particle at the surface introduced as plasmons. The transmittance, reflectance and absorption of the device was analyzed using microwave studio wave, computer simulated technology. We measured the absorption efficiency and compare it with the absorption pattern of CoO-ATO thin film and nanofiber layer.

The magnification power of Hitachi S-800 is 300,000 times the actual size of the particle. Very fine beam of electron scans over the specimen to generate the magnified image. At the surface of the specimen the electrons are scattered and afterward composed to produce an image. The machine has 2nm resolution. It accepts samples of 25 millimeter diameter by 20 millimeter height. If the sample is nonconductive then an layer of gold palladium (ultra-thin) is coated to the sample using A Hummer X sputter coater. This process prevents charging of electrons.

The sample of Cobalt oxide solution used in this thesis was analyzed using SEM.

4.4. Ellipsometry

In this thesis Rudolph Auto ALIII Null Ellipsometer having a resolution of 0.1 nanometer up-to two layers is used for obtaining the optical characterization of the novel material, CoO-ATO. Rudolf Ellipsometer is used for measuring the index of refraction and the transparent film thickness. The Rudolf Ellipsometer used for thesis in NREC, at University of South Florida uses one laser beam of wavelength λ=638.2nm.

When an incident beam of light hits the surface of the sample a part of it is reflected some refracted and a portion of it is transmitted. Change of polarization light after being reflected from the surface of the sample is measured by ellipsometry. The equipment measures values which are recorded as Δ and . The obtained values are correlated to Fresnel reflection coefficients ratio. As ratio of two values is measured in ellipsometry, the measured values obtained are precise. A complex number is obtained from the ratio which additionally yields the phase information. [19]

4.5. Refractive Index Measurement of CoO-ATO

The Rudolph Ellipsometer measured the refractive index of the thin film of CoO-ATO with diminutive standard deviation. The real part of the complex refractive index is 1.545 with extinction coefficient 0.068 at λ=632.8nm.

The refractive index was measured then using Sopra Spectroscopic Ellipsometer ES 4G. Cobalt oxide antimony doped tin oxide shows dispersive nature in the range of visible spectrum.

The following table shows the real and imaginary part of the refractive index obtained using ellipsometry.

Table 4.1: Refractive Index of CoO-ATO across the visible spectrum

Frequency (Hz)	**n**	**k**		**Frequency (Hz)**	**n**	**K**
8.57E+14	1.580748	0.409308		5.00E+14	1.50626	0.383945
8.33E+14	1.573784	0.356957		4.92E+14	1.503842	0.409926
8.11E+14	1.555642	0.354194		4.84E+14	1.504305	0.374454
7.89E+14	1.552619	0.345089		4.76E+14	1.496773	0.367405
7.69E+14	1.556517	0.354759		4.69E+14	1.494514	0.335042
7.50E+14	1.535832	0.36656		4.62E+14	1.492598	0.36782
7.32E+14	1.537883	0.361038		4.55E+14	1.489995	0.339408
7.14E+14	1.527165	0.361512		4.48E+14	1.475374	0.352766
6.98E+14	1.530031	0.355847		4.41E+14	1.502699	0.343499
6.82E+14	1.531308	0.345078		4.35E+14	1.484886	0.365417
6.67E+14	1.531567	0.343071		4.29E+14	1.478083	0.362596
6.52E+14	1.524342	0.346114		4.23E+14	1.482968	0.42966
6.38E+14	1.519839	0.347926		4.17E+14	1.459432	0.466955
6.25E+14	1.530565	0.359216		4.11E+14	1.440916	0.520515
6.12E+14	1.518527	0.365619		4.05E+14	1.433436	0.525135
6.00E+14	1.529964	0.35695		4.00E+14	1.422648	0.58114
5.88E+14	1.511256	0.346488		3.95E+14	1.405527	0.593234
5.77E+14	1.519249	0.359488		3.90E+14	1.401552	0.603808
5.66E+14	1.500164	0.363596		3.85E+14	1.381981	0.663803
5.56E+14	1.509407	0.380476		3.80E+14	1.392105	0.624652
5.45E+14	1.514883	0.381926		3.75E+14	1.386026	0.70657
5.36E+14	1.498919	0.369322		3.70E+14	1.368083	0.66166
5.26E+14	1.506147	0.341732		3.66E+14	1.394243	0.709533
5.17E+14	1.506477	0.371935		3.61E+14	1.375207	0.641783
5.08E+14	1.502753	0.367606		3.57E+14	1.37761	0.772687

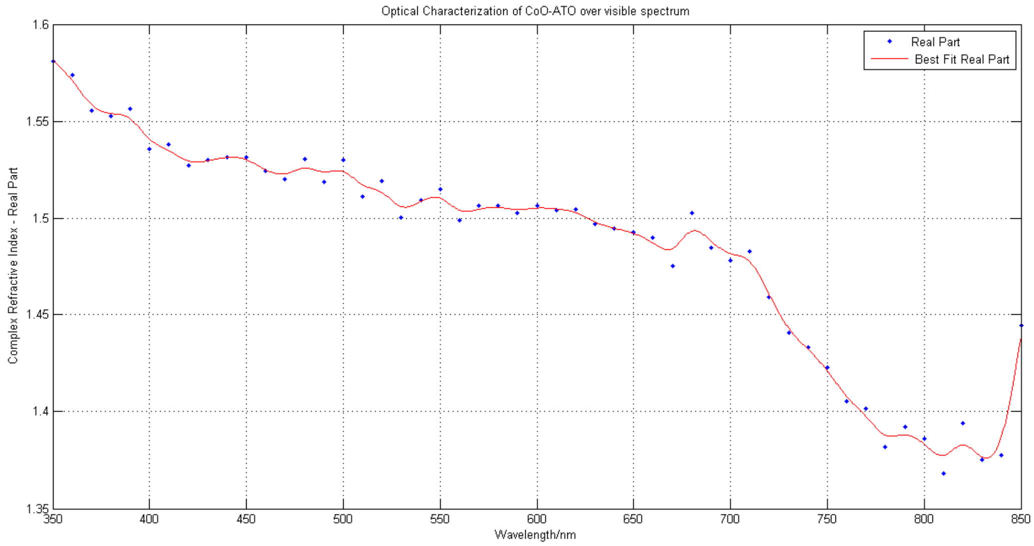


Figure 4.8: Refractive index of CoO-ATO over visible spectrum

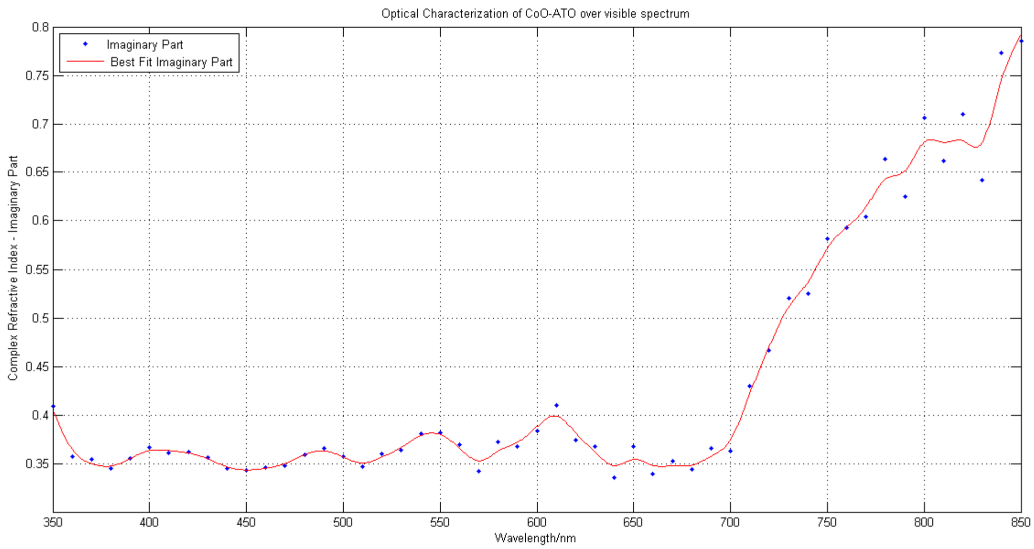


Figure 4.9: Extinction coefficient of CoO-ATO over visible spectrum

CHAPTER 5: MODELING AND SIMULATION OF OPTOELECTRONIC DEVICE

5.1. Proposed Model

This thesis models a silicon solar cell with a novel conducting oxide layer of CoO-ATO as an antireflective coating layer. The CoO-ATO layer is modeled as a thin film and nanofiber membrane. The model is generated in microwave studio CST (Computer simulated technology) and from the simulated result the transmission and reflection coefficient is obtained to plot an absorption and efficiency profile and hence obtaining the absorption efficiency for the simulated optoelectronic device.

5.2. Construction of Silicon Substrate

The silicon substrate is modeled and generated in microwave studio CST for analyzing the absorption of the film without modeling any antireflective coating at the top so that a control reference for analysis is developed. The model of the silicon thin film structure is presented in the Figure 5.1.

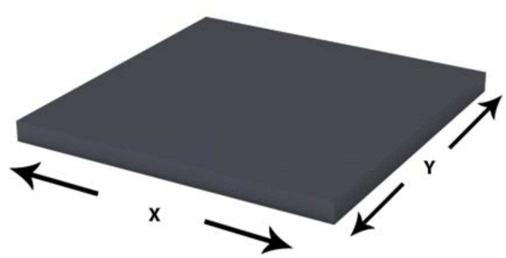


Figure 5.1: Silicon substrate

The thickness of the silicon substrate used in the developed model has a dimension of 3μm thickness (z) and its width (y) and length (x) is 0.50μm.

Table 5.1: Material parameter of the silicon substrate used as reference

Material	Silicon (Loss free)
Type	Normal
Epsilon	11.9
Mu	1
Rho	2330 [kg/m3]
Therm. cond.	148 [W/K/m]
Heat cap.	0.7 [KJ/K/Kg]
Diffusivity	9.07419e-005 [m2/s]
Youngs Mod.	112 [KN/mm2]
Poiss. Ratio	0.28
Thermal Exp.	5.1 [1e-6/K]

Software simulation obtained the scattering parameters (Transmission and reflection coefficient) of the reference silicon substrate which are used for obtaining the absorption profile of the material. Using the absorption profile of the silicon, spectral irradiance and the ultimate efficiency equation the absorption efficiency of the silicon substrate is computed.

Within the range of 1.1eV to 4.13eV corresponding to 265 THz to 1000 THz silicon is dispersive in nature. To construct the model of silicon substrate optical constant which is experimentally measured is used [13].

The optical constants of the material are worked out using dispersion model (nth order) by calculating the ϵ' and ϵ'' using complex refractive index.

5.3. Modeling of Optoelectronic Device with Thin Film Antireflective Coating

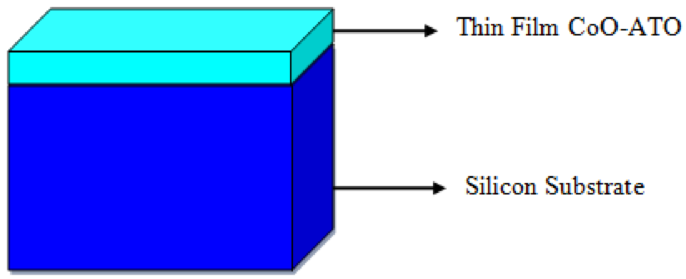


Figure 5.2: Unit cell of thin film antireflective coating over the reference model

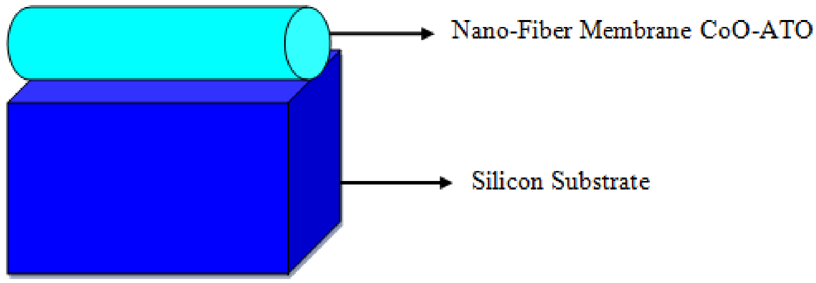


Figure 5.3: Unit cell of nanofiber membrane antireflective coating over the reference model

Design and simulation of the model of the optoelectronic device has been done under computer simulated technology. The reflection and transmission coefficient of models are obtained and analyzed. A plane wave source has been used which is polarized to reproduce the solar illumination with boundary conditions, Y= Magnetic (Ht=0), X=Electric (Et=0) and Z= open. [14]

The nth orde dispersive model reveals the fact that novel material, CoO-ATO is dispersive in nature across the visible spectrum. Figure 5.4 shows the electric dispersion of the material across the visible spectrum.

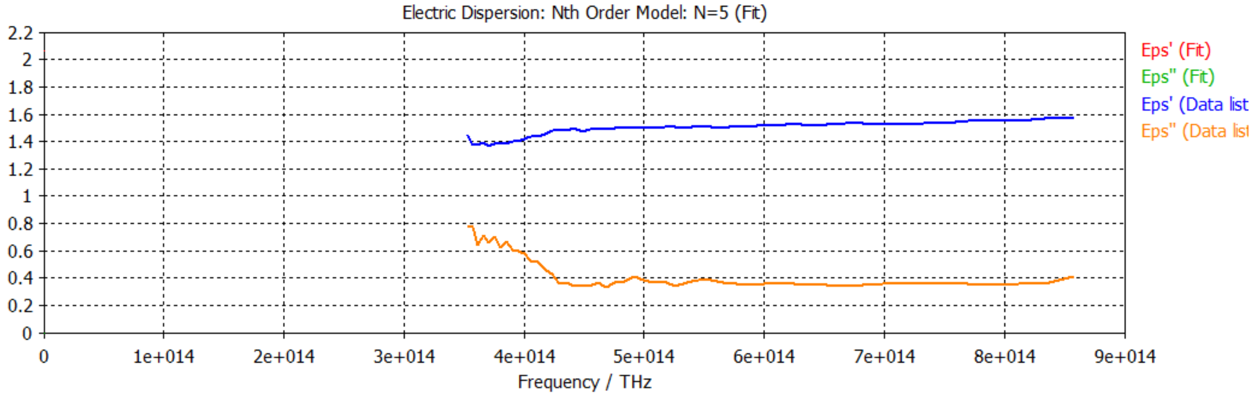
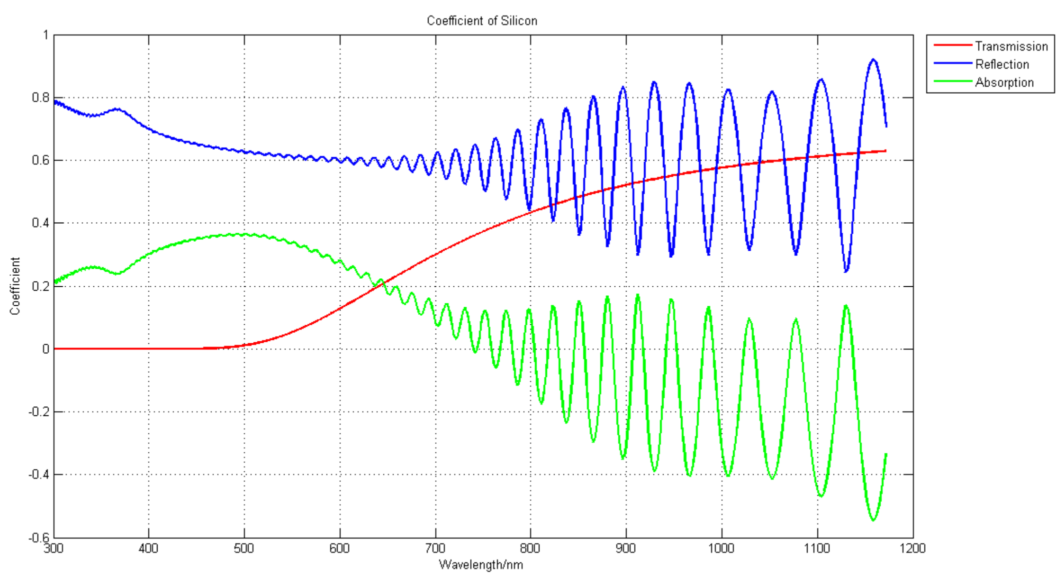


Figure 5.4: Electric dispersion of CoO-ATO

CHAPTER 6: COMPARATIVE ANALYSIS OF THE ABSORPTION EFFICIENCY OF OPTOELECTRONIC DEVICE WITH THIN FILM AND NANO FIBER MEMBRANE ANTI-REFLECTIVE COATING

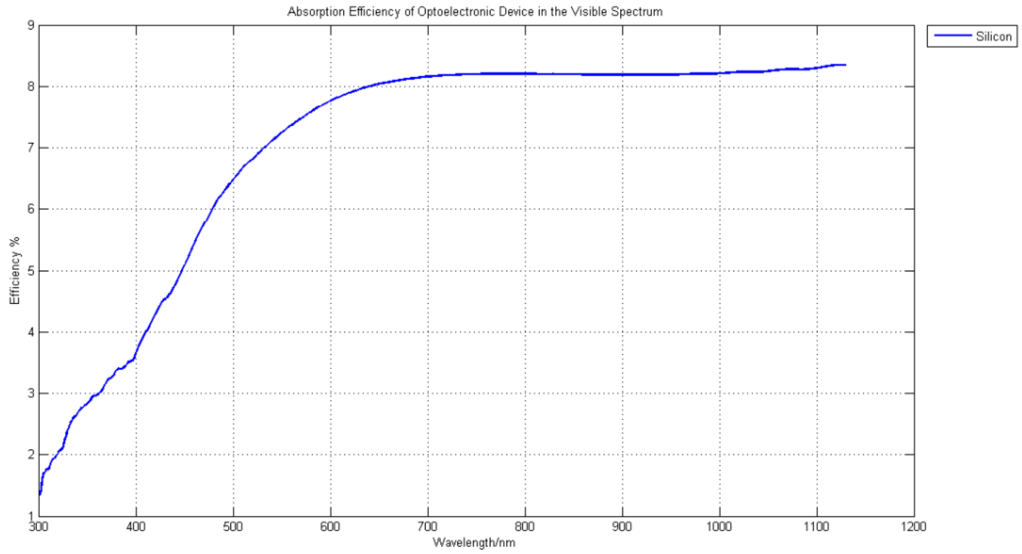
This chapter presents the results of the findings of the comparative analysis of absorption, reflection and transmission coefficient obtained from the simulations of the 2D-3D model of CoO-ATO. The absorption profiles are compared and the compared graphical data are presented. The section also includes the absorption efficiency profiles of different models for the thesis.

From the simulation the transmission coefficient, reflection coefficient and absorption are given in the figure (a). Further, efficiency is calculated and generated graphically which is given in figure (b). The efficiency of thin film Si solar cell is 8.2084%.



(a) Transmission coefficient, reflection coefficient and absorption

Figure 6.1: Thin film silicon solar cell



(b) Efficiency

Figure 6.1: (Continued)

To the reference simulated model a layer of antireflective coating in the form of thin film is added. The new modeled optoelectronic device with the novel material is simulated (unit cell) and the scattering parameters are obtained. From the transmission and reflection coefficient the absorption profile of the thin film is obtained using energy balance equation. Figure shows the absorption of the optoelectronic device modeled in computer simulated technology.

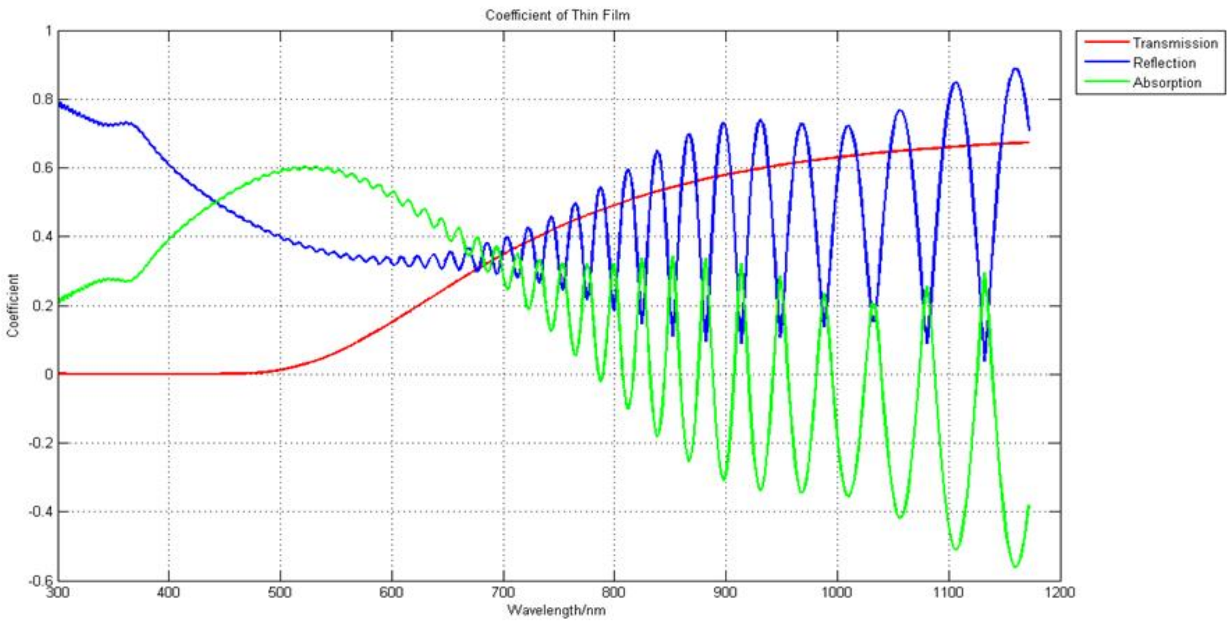


Figure 6.2: Transmission coefficient, reflection coefficient and absorption of CoO-ATO thin film

The procedure is repeated. The thin film antireflective coating in the reference substrate is replaced by the nanofiber membrane. A unit cell is simulated. The scattering parameters are obtained from the simulated results. From the transmission and reflection coefficient the absorption profile is obtained. The absorption efficiency is computed from the obtained data using energy balance equation. Figure shows the absorption of the optoelectronic device modeled in computer simulated technology.

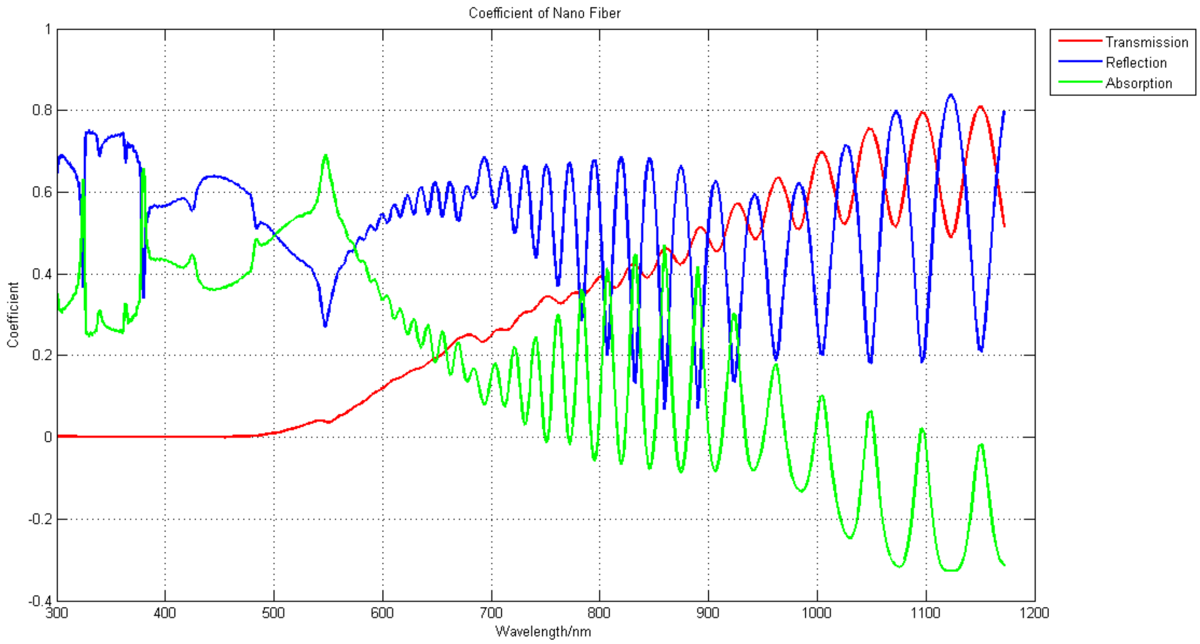


Figure 6.3: Transmission coefficient, reflection coefficient and absorption of CoO-ATO nanofiber membrane

Using the absorption profile and the spectral irradiance the absorption efficiency is computed and plotted within the visible spectrum. Figure shows the absorption efficiency of optoelectronic device with antireflective coatings in the form of thin film and nanofiber membrane of the novel material compared to the reference model containing no silicon substrate.

Table 6.1: Summary of absorption efficiency

Type of Antireflective Coating	**Efficiency (%)**
Thin film	8.7521
Nanofiber membrane	8.2681

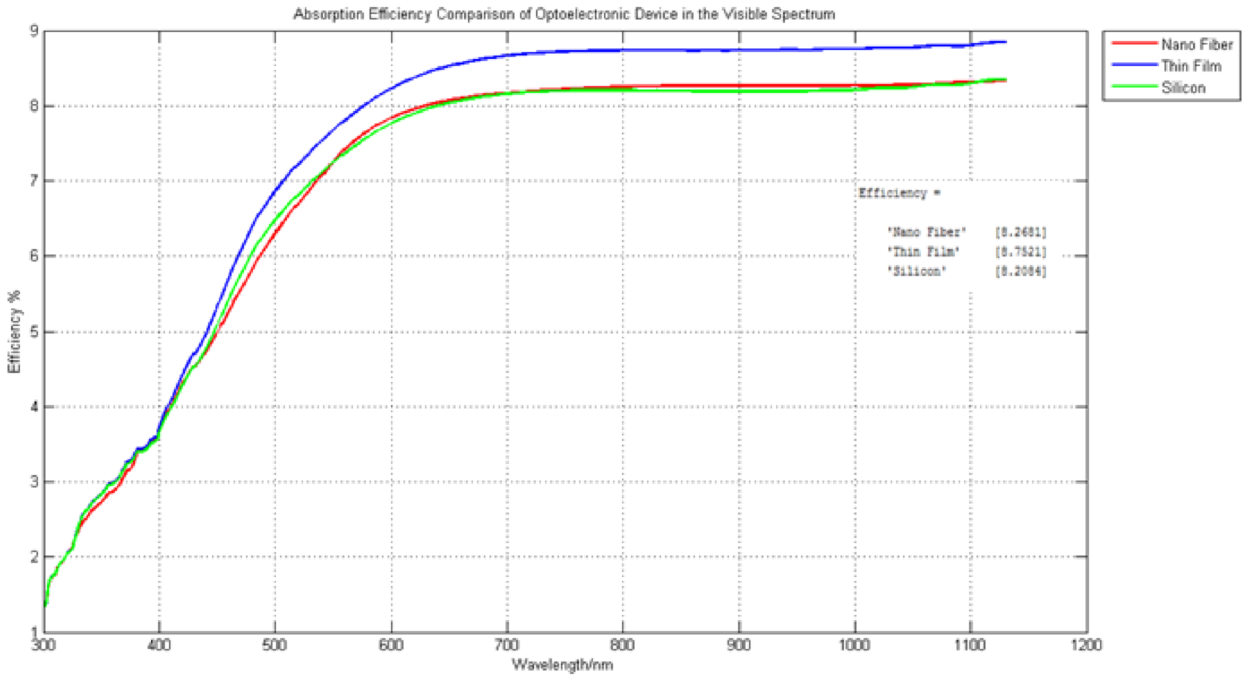


Figure 6.4: Absorption efficiency of optoelectronic device with no antireflective coating (Silicon), and optoelectronic device having antireflective coating in the form of thin film and nanofiber membrane of CoO-ATO

CHAPTER 7: CONCLUSION AND FUTURE WORK

This section presents the outcome of the findings from the research and proposes new set of data for the novel material which could be used in further investigation. It summarizes the findings and proposes the best form of the material that could be used for modeling the optoelectronic device with enhanced efficiency. It also states the proposed future work in the field.

The purpose of the research was to make an optical characterization of the novel material, CoO-ATO from the analysis of the result suggesting if the material is a good choice as an antireflective coating that could be implemented as a layer in solar cells for improved performance.

The thesis characterized the optical constant of the material (refractive index) over visible spectrum. From the analysis of the experimental result, the novel material is found to be dispersive over a broad range of visible spectrum. The thesis also presents the extinction coefficient profile that gives us an idea of the absorbance of the visible material across the visible spectrum.

Form the analysis of the optical characterization of the material an optoelectronic device is modeled having a layer of the antireflective coating of the material. The antireflective coating was modeled in the form of nanofiber membrane and thin film.

The absorption efficiency of all models is presented and introducing a layer of the antireflective coating in the model showed enhancement in absorption efficiency. Thin film is more efficient compared to the nanofiber membrane.

We can conclude:

1. Antireflective coating of the novel material CoO-ATO in the form of thin film and nano fiber membrane have the potential to enhance device efficiency and reduce the cost of harvested solar energy.
2. Modeling a layer of CoO-ATO thin film and nanofiber membrane, over a 3μm thin film Si substrate, showed improved optical absorption and absorption efficiency of the optoelectronics device over the visible spectrum.
3. The model that has been developed investigates the effect of changing the anti-reflective coating from thin film to nanofiber membrane located adjacent to the Si substrate. Change in the type of anti-reflective coating showed difference in light absorption compared to bare silicon substrate.

7.1. Future Work

For future investigation we want to use the optical characterization to develop a tandem plasmonic solar cell having CoO-ATO as an antireflective coating and introduce metal nano particle to trap light and increase optical path length enhancing the overall device efficiency.

The modeling of the optoelectronic device is done using computer simulated technology. The scattering parameters obtained contained ripples which can be optimized by adjusting parameters in the model. Future investigation will take consideration and optimize the design to minimize losses.

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APPENDIX A: CST WORKING MODULE

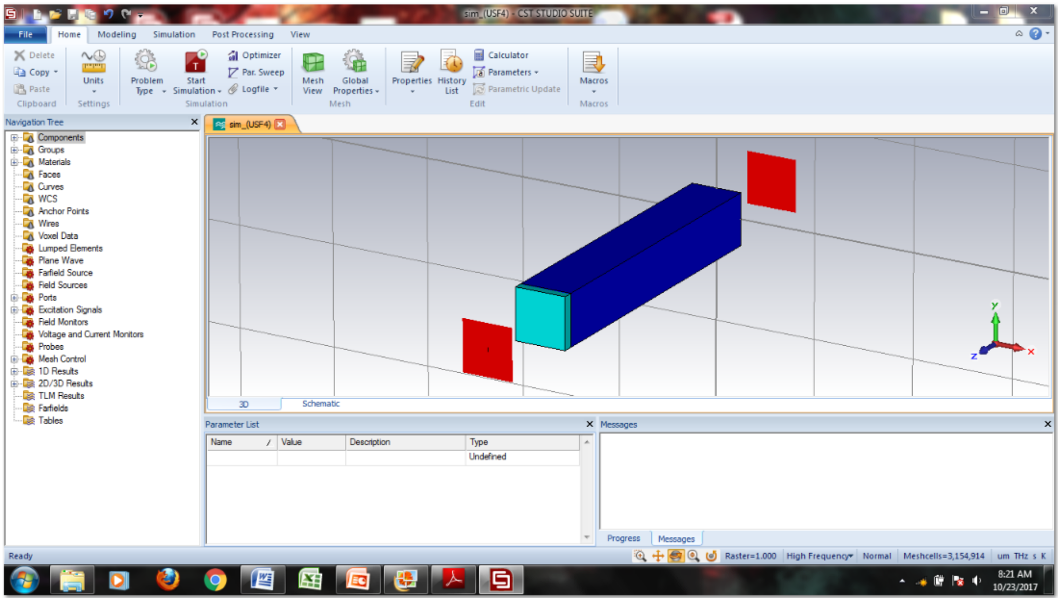

Figure A.1: CST Microwave Studio Suite (Design window)

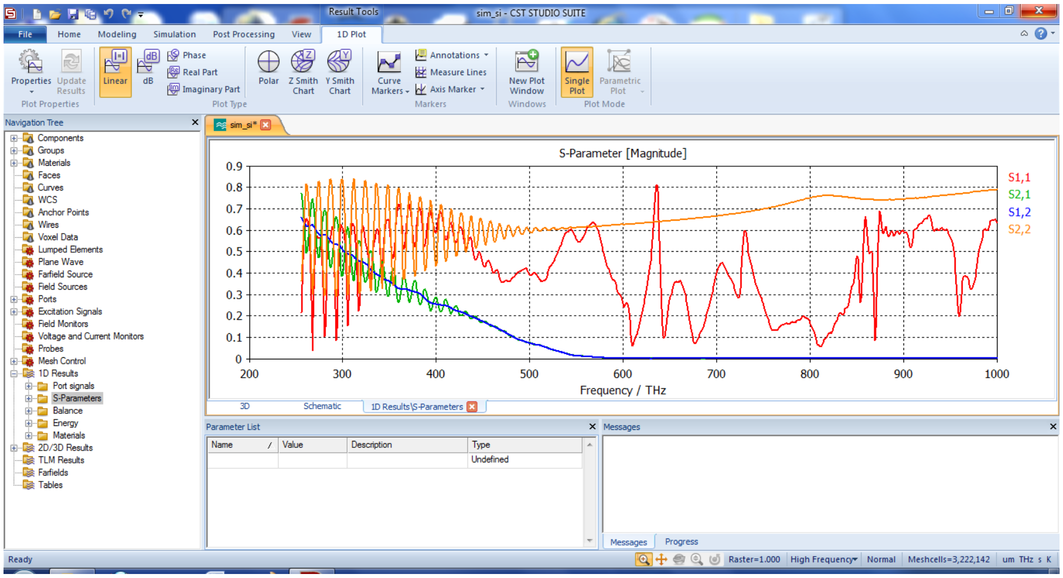

Figure A.2: CST Microwave Studio Suite (S-parameter window)

APPENDIX B: GLOSSARY OF TERMS

D	Dielectric Displacement
H	Magnetic Field
E	Dielectric Field
B	Magnetic Induction
n	Refractive Index
k	Extinction Coefficient
G_λ	Solar spectrum
A	Absorption factor
R	Reflection Factor
T	Transmission Factor
η	Ultimate Efficiency
λ	Wavelength
λ_G	Wavelength Corresponding to Band gap
I(λ)	Spectral Irradiance
A(λ)	Overall Absorption
OPL	Optical Path Length
ARC	Anti-Reflective Coating
SEM	Scan Electron Microscopy

APPENDIX C: SOFTWARE

1. CST MICROWAVE STUDIO SUITE 2013
2. MATLAB 2010
3. Microsoft Word

ABOUT THE AUTHOR

Ridita Rahman Khan is a Bangladeshi and she completed her bachelor in Electrical and Electronics Engineering. During her bachelor degree she was a research assistant and her field of expertise in research was photovoltaics technology.

She moved in United States on January 2016 to pursue her master in Electrical Engineering. During her Master's program she majored in microelectronics. She started work in Advance Material Bios and Integration Research Laboratory under supervision of Dr.Sylvia Wilson Thomas. She worked with the solar research team during Masters and in her thesis she characterized the optical property (index of refraction) of a novel material, Cobalt Oxide Antimony doped Tin Oxide (CoO-ATO). Using the optical characterization she developed an anti-reflective coating of an optoelectronic device through simulation which enhanced the absorption efficiency of the device within the range of visible spectrum. The developed model will now be used to develop a tandem solar cell with enhanced overall efficiency to harvest renewable energy reducing the usage of conventional fossil fuels

She wishes to contribute in the field of advanced photovoltaic technology developing better model for harvesting low cost high efficient solar cells.