Plasma -Assisted Carbon Nanotube for Solar cell application

A thesis submitted in partial fulfilment of the requirements for the award of the degree of

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in
Physics

By

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CANDIDATE'S DECLARATION

We, **SURAJ KUMAR SINGH, Roll No 2K22/MSCPHY/42** and **ISHU SHARMA Roll No 2K22/MSCPHY/53**. Student of **M.Sc. Physics** hereby declares that the project Dissertation titled ***"Plasma- Assisted Carbon Nanotube for Solar cell application".*** Which is submitted by us, under the supervision of **Prof. SURESH C. SHARMA**, to the Department of Applied Physics, Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of the degree of Master of Science is original and not copied from any source without proper citation. This work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or other similar title or recognition.

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CERTIFICATE

I, hereby certify that the Project Report titled " ***Plasma Assisted Carbon Nanotube for Solar cell application***" Which is submitted by **SURAJ KUMAR SINGH**, **Roll No 2K22/MSCPHY/42, and ISHU SHARMA, Roll No 2K22/MSCPHY/53** Department of Applied Physics, Delhi Technological University, Delhi in partial fulfilment of the requirement for the award of the degree of Master of Science, is a record of the project work carried out by the student under my supervision. To the best of my knowledge this work has not been submitted in part or full for any Degree or Diploma to this University or elsewhere.

SUPERVISOR

Place: Delhi
Prof. Suresh C. Sharma

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Place: Delhi **Suraj Kumar Singh**

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Chapter 1: Introduction

1.1 Solar Cell Introduction

Solar cells, also known as photovoltaic cells, convert sunlight into electric current from photovoltaic effect. The principle of solar cells involves the birth of an electric current when certain materials are exposed to light.

1.1.1 Principle of Solar Cell

Solar cell works upon Photovoltaic effect can be say it is little bit similar to photoelectric effect. In photovoltaic effect when incident Light falls on material then free electrons of that metal start moving within the material while in Photoelectric electron left the metal surface completely this effect is called Photovoltaic effect.

1.1.2 Construction of Solar Cell

It consists of a P-N Junction Diode in which N region has small thickness 0.3 micrometre and P region has large thickness 300 micrometre. N region is made thin so that light falling on the solar cell is not absorbed significantly before reaching the junction. On the top of silicon layer metallic fingers are deposited. This is called Front contact. The bottom of P type silicon layer is coated with metal(copper) this is called back contact.

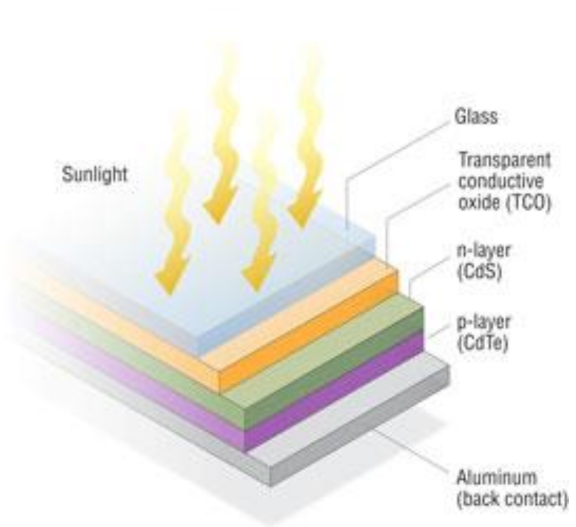

Fig. 1.1 Schematic Diagram of Solar Cell

1.1.3 Working of Solar cell

Photovoltaic effect can be explained by When selected materials, mainly semiconductors like silicon, are exposed to light, particles of light strike the surface of the material and the energy from these photons is absorbed by electrons available in the material, causing them to be excited and move to a higher energy state. The absorption of light energy makes electron-hole pairs. An electron is excited to an excited energy level (conduction band), and left positively charged holes and in the initial state (valence band).So there is an internal electric field established by the semiconductor material. This electric field helps to separate the electron and hole pairs and Due to this internal electric field, the excited electrons are attracted in direction of electron on collector electrode mainly the n-type semiconductor, while the holes are driven towards the hole-collecting electrode mainly the p-type semiconductor and the motion of electrons and holes creates an electric current.

1.1.4 Efficiency Calculation for solar cell

The Photo Current Density of semiconducting device i.e. Solar Cell given by

$$J_{\text{sc}} = q \int \text{QE}(E) b_{\text{s}}(E) dE,$$

Where, q = Charge on electron can be denoted by e also have value 1.6×10^{-19}c

$b_s(E)$ = Flux Density of Incident Photons

QE(E) = Probability of incident light particles with energy E which is given to the electron to the Load Circuit.

A dark current also found in solar cells denoted by $J_{dark}(V)$ at an external voltage (V) can be calculated by:

$$J_{\text{dark}}(V) = J_0(\mathrm{e}^{qV/nk_{\text{B}}T} - 1),$$

Where, J_0 = constant

N = Ideality factor

K_b= Boltzmann constant

T = Absolute temperature in kelvin

Now, Net current density is equal to the addition of photocurrent density and dark current density. And dark current having same direction. So net current density will be:

$$J = J_0\left(\mathrm{e}^{qV/nk_{\text{B}}T} - 1\right) - J_{\text{sc}}$$

When circuit is open, $J_{dark}(V)$ = Jsc. Equation for open circuit voltage (Voc) will be:

$$V_{oc} = \frac{kT}{q} \ln\left(\frac{J_{sc}}{J_0} + 1\right).$$

In a real solar cell, we have materials resistance also, So the resistance of all contact terminals, also the leakage current gives energy decrement .These resistances are electronically similar to two parasitical resistances connected in series (R_s) and connected in parallel (R_{sh}). So, the current density will be

In a real solar cell, we have materials resistance also, So the resistance of all contacts, and the leakage current gives power decrement .These resistances are electronically similar to double parasitical resistances connected in series (R_s) and connected by parallel method (R_{sh}). So, the current density will be :

$$J = J_0\left(e^{q(V-JAR_s)/nk_BT} - 1\right) + \frac{V - JAR_s}{AR_{sh}} - J_{sc}$$

Where

A= Solar Cell Effective area

Definition Of Fill Factor (FF):

The Fill factor is explained like it is division of product of $J_m.V_m$ and J_{sc} .Voc respectively

$$\mathrm{FF} = \frac{J_m V_m}{J_{sc} V_{oc}}.$$

Solar cell efficiency (η) with incident light power density (P_{in})

$$\eta = \frac{\mathrm{FF} \times V_{OC} \times J_{SC}}{P_{in}} \times 100$$

1.2 Carbon nanotube Based Solar cell

1.2.1 Carbon nanotube (CNT)

Carbon nanotubes (CNTs) invented by Japanese Scientist Sumio Iijima in 1991.CNT are very good conductors of electricity, it is extremely flammable due to Presence carbon.

There are many types of CNT available like Single wall Carbon nanotube and Multi wall carbon nanotube. CNT are made by folding Graphen sheet if we fold cylindrically a single sheet of graphene then we got Single Wall CNT and when we fold multiple graphene sheet then we got Multi wall CNT.

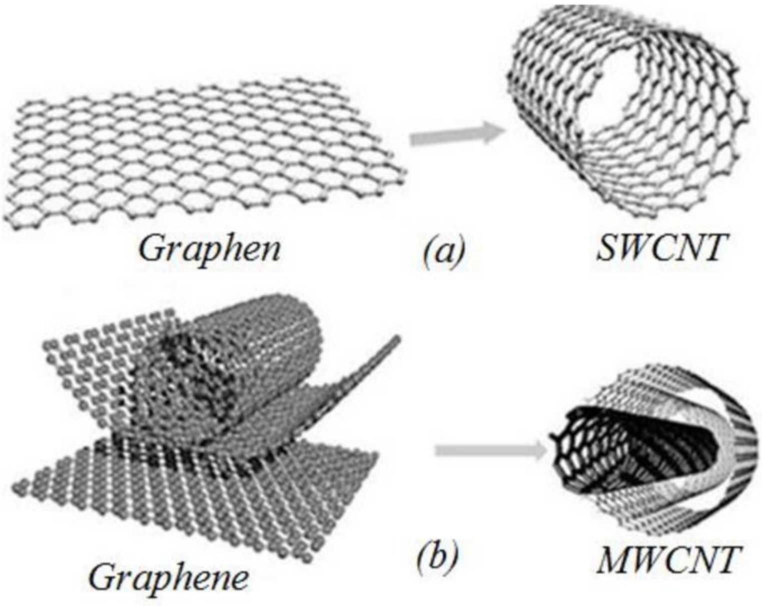

Fig. 1.2 Different Types of CNTs

1.2.2 CNT Implements in Solar Cells

Here we Use Carbon Nanotube in place anode of the Solar cell and in future Carbon Nanotubes can replace ITO, Active layers etc. Whenever CNTs would be used then the show improvement in efficiency due to its very good conductor nature. CNTs based Solar cell can improve efficiency up to 27%.

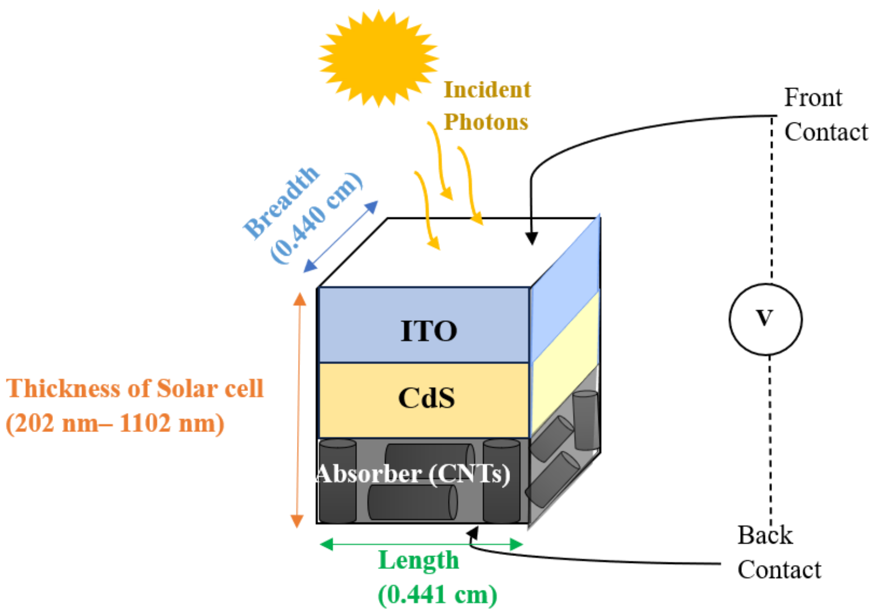

Fig. 1.3 CNT implement in single solar cell

1.3 Growth of Carbon Nanotubes using plasma

1.3.1. Main techniques;

A. Arc discharge
B. laser ablation
C. Chemical Vapour deposition Method

Here, we focus on only CNT grown from PECVD techniques

1.3.1c Chemical Vapor Deposition (CVD) Method

Chemical Vapor Deposition (CVD) is a method used to produce thin films and coatings by the chemical reaction of gaseous precursors on a substrate surface. This process is widely employed in various industries for applications such as semiconductor manufacturing, thin film deposition, and surface modification. Here's an overview of the CVD method.

Carbon nanotube growth by PECVD:

Plasma enhance chemical vapour deposition method is a technique that is uses in various industries such as microelectronics and material sciences to deposit thin film on substrate. The process involves the uses of plasma to enhance the chemical reactions that lead to the deposition of the desired materials. Here is a more detailed explanation of this process.

1. Introduction of Precursors

Volatile precursors gases are introduced into a vacuum chamber where the substrate is located. These precursors are the source materials for the thin film to be deposited.

2. Creation of Plasma

A plasma is generated in the chamber. Plasma is a state of matter in which a gas become ionized, meaning that some of the atoms or molecule loose or gain electrons and become charged particle (ion and electrons). This is a typically achieved by applying a high frequency electric field (RF and Microwave energy) to the gas.

3. Chemical Reactions

The energetic species within the plasma, such as ions, electrons and radicals interact with the precursor's gases. this interaction induces chemical reactions that lead to the formation of solid or liquid thin films. Plasma serves to break down the precursor molecules and enhance the reactivity of the species involved.

4. Deposition

The reaction by products and newly formed materials are deposited thin films . The properties of thin films , such as thickness and compositions can be changed by adjusting knobs of machine such as gas flow rate Plasma enhance chemical vapour deposition method is a technique that is uses in various industries such as microelectronics and material sciences to deposit thin film on substrates .The process involves the uses of plasma to enhance the chemical reactions that lead to the deposition of the desired materials and pressure.

Setup of PECVD Technique:

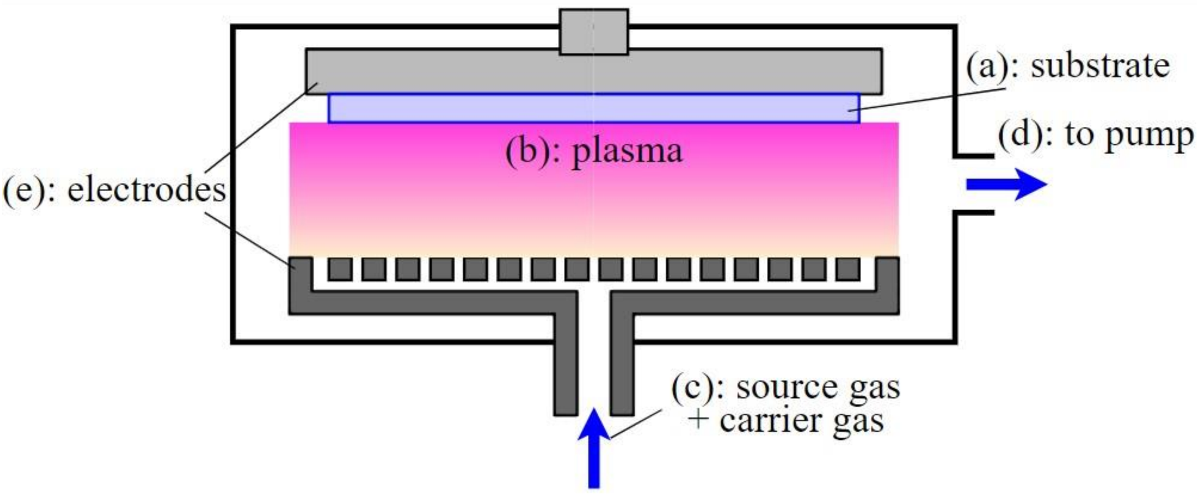

Fig. 1.4 Schematic Diagram of PECVD Machine

1.4 Application of CNT based Solar cells

CNTs are known for their flexibility and lightweight nature. Integrating CNTs into solar cells can lead to the development of flexible and lightweight solar panels. This is particularly useful in applications where traditional, rigid solar panels are not practical, such as on curved surfaces or for portable solar devices. CNTs can be engineered to be transparent, allowing for the creation of transparent solar cells. These cells could be incorporated into windows or other transparent surfaces to generate electricity without obstructing light and visibility. This application is relevant for building-integrated photovoltaics (BIPV). CNT-based solar cells may exhibit better tolerance to high temperatures compared to traditional silicon-based solar cells. This could make them suitable for environments with elevated temperatures, such as in space applications or concentrated solar power systems.

1.5 Advantages of CNT Based Solar cell

(A) The unique electronic properties of CNTs may contribute to improving the efficiency of solar cells up to 27%.

(B) Carbon nanotubes can be produced through various methods, and researchers are investigating scalable and cost-effective manufacturing processes for CNT-based solar cells. If successful, this could contribute to reducing the overall cost of solar energy production.

1.6 Disadvantages of CNT Based Solar Cell

(A)Since CNT are used and they are highly flammable so they are not firing resistance.

(B)CNT manufacturing is little bit tough to grow so they have consisted less production speed.

1.7 SCAPS Software

Solar cell capacitance software (SCAP) is a solar cell simulator. Which is developed by the Department of Electronics and information system(ELIS) of the University of Gent,Belgium.

It is used to simulate to device and analyze its Photovoltaic values and also Current Densities, Open circuit voltage and efficiency etc.

The Scientists who have invented this are

Alex Niemegeers, Mark Burgelman, Koen Decock, Stefaan Degrabe, John Verschraegen.

1.7.1 Interface of SCAPS

Fig. 1.5 Interface of SCAPS Software

1.7.2 Software References

References for the program and its algorithm can be found in the following literature:

[1]. M. Burgelman, P. Nollet and S. Degrave, "Modelling polycrystalline semiconductor solarcells", *Thin Solid Films*, **361-362**, 527-532 (2000).

[2]. M. Burgelman, K. Decock, S. Khelifi and A. Abass, "Advanced electrical simulation ofthin film solar cells", *Thin Solid Films*, **535** (2013) 296-301.

[3]. K. Decock, P. Zabierowski, M. Burgelman, "Modeling metastabilities in chalcopyrite-based thin film solar cells", *Journal of Applied Physics*, 111 (2012) 043703.

[4]. K. Decock, S. Khelifi and M. Burgelman, "Modelling multivalent defects in thin filmsolar cells", *Thin Solid Films*, 519 (2011) 7481-7484.

[5]. M. Burgelman and J. Marlein, "Analysis of graded band gap solar cells with

SCAPS", *Proceedings of the 23rd European Photovoltaic Solar Energy Conference*, (Valencia,E, september 2008), 2151-2155, (2008).

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[7]. S. Degrave, M. Burgelman, P. Nollet, "Modelling of polycrystalline thin film solar cells:new features in SCAPS version 2.3", *Proceedings of the 3rd World Conference on*

Photovoltaic Energy Conversion (Osaka, Japan, may 2003), pp. 487-490, WCPEC-3, Osaka,2003.

[8]. A. Niemegeers and M. Burgelman, "Numerical modelling of ac-characteristics of CdTeand CIS solar cells", *Proc. 25nd IEEE Photovol-taic Specialists Conference* (Washington D.C., april 1996), pp. 901-904, IEEE, New-York, 1996.

Chapter 2: Modelling and simulation of Plasma Assisted Carbon Nanotubes (CNTs) based Solar cell

2.1 Literature Review

In the beginning of our research, we have read the following published research papers under the guidance of our supervisor.

[1] *Applications of Carbon Nanotubes in Solar Cells By Feijiu Wang and Kazunari Matsuda.*

[2] *Mansha Kansal, · Suresh C. Sharma, Plasma-based nanoarchitectonics for vertically aligned dual-metal carbon nanotube field-effect transistor (VA-DMCNFET) device: effect of plasma parameters on transistor properties.* *https://link.springer.com/article/10.1007/s00339-021-05096-2*

[3] Introduction to plasma physics by F.Chain

[4] *8. Laura Wieland, Han Li, Christian Rust, Jianhui Chen,* and Benjamin S. Flavel*Carbon Nanotubes for Photovoltaics: From Lab to Industry*
https://onlinelibrary.wiley.com/doi/10.1002/aenm.202002880
https://www.nature.com/articles/ncomms7305

[5]. *Severin N. Habisreutinger, Tomas Leijtens, Giles E. Eperon, Samuel D. Stranks, Robin J. Nicholas,and Henry J. Snaith**
Carbon Nanotube/Polymer Composites as a Highly Stable Hole Collection Layer in Perovskite Solar Cells
https://pubs.acs.org/doi/10.1021/nl501982b

[6]. *Brian J. Landi1, Ryne P. Raffaelle1*,y, Stephanie L. Castro2 and Sheila G. Bailey3*
Single-wall Carbon Nanotube–Polymer Solar Cells
https://onlinelibrary.wiley.com/doi/10.1002/pip.604

[7]. *Utkarsh Kumar1,Samiksha Sikarwar1,Rakesh K. Sonker1, B. C. Yadav1*
Carbon Nanotube: Synthesis and Application in Solar Cell
https://link.springer.com/article/10.1007/s10904-016-0401-z

Table 1 Parameters and Symbols used in the present work

Parameters	**Symbols**
Effective area of the Solar cell	A
Resistances in series	Rs
Surface recombination velocity for electrons	Se
Electron concentration	N
Current density	J
Recombination rate of Holes	R_p
Ideality factor	n_o
Resistances in Parallel	R_{sh}
Reverse Saturation Current density	J_o
Carbon Nanotubes	CNTs
Recombination rate of Electrons	R_n
Length of CNT	L
Radius of CNT	R
Power Conversion Efficiency	PCE
Electron Temperature	T_{eo}
Ion Temperature	T_{io}
Debye length	λ_D
Solar irradiance	P_{in}
Generation rate of Electrons	G_n
Absolute temperature	T
Electronic charge	q
Electron Density	n_{eo}
Surface recombination velocity for holes	Sh
Ion Density	n_{io}
No. of Carbon Nanotubes (CNTs)	N
Efficiency of Solar cell	η
Power Output	P_{out}
Indium tin oxide	ITO
Open circuit voltage	V_{OC}
Electron current density	J_n
Generation rate of Holes	G_p
Air mass spectrum	AM
Photocurrent density	J_{SC}
Conduction band	CB
Boltzmann's constant	K_B
Valance band	VB
Hole concentration	p
Metal work function	φ
Transparent conductive oxide	TCO
Hole current density	J_p
Quantum efficiency	QE
Surface Potential	V_S
Thickness of Absorber layer	t
Fill factor	FF

2.2 INTRODUCTION

Solar cell is a photovoltaic device that converts light radiation into electric energy [1]. It works same as P-N based photodetector. When sunlight is incident on a Solar cell then electrons of the conduction band (CB) jump to the valance band (VB) then holes are created in the conduction band that cause current flow in the Solar cell [2]. This electron and hole generated current is called photocurrent [3-7]. The photovoltaic conversion efficiency of Solar cell is up to 1 to 5 % [8,1]. Solar cell photovoltaic conversion efficiency (PCE) depends upon photocurrent density, fill factors (FF) and input power irradiance (P_{in}) and open circuit voltage (Voc) [9]. There are various types of Solar cells e.g., thin film based Solar cells, perovskite operating Solar cells, dye sensitized operating Solar cells etc. [2]. The perovskite Solar cells have photovoltaic conversion efficiency up to 22.1 % [10] but it is not much stable under light illumination condition. Researchers noticed that when Carbon Nanotubes (CNTs) are used in Solar cells then PCE of CNTs based Solar cell increases up to 1.3% to 30% [9]. Since, the structure of CNTs based Solar cells is same as single P-N junction Solar cell where the CNTs is uses at the place of P or N type junction [2, 10]. CNTs are grown firstly by Japanese scientist Sumio Ijima in 1991 [11-13]. CNTs are highly conductive and higher than Copper with an extremely high surface area, it is very strong because of the covalent SP^2 bond between individual Carbon atoms [14]. The band gap of CNT is 0.1 eV to 2 eV [14-17]. The basic structure of CNTs have 3 types: 1. Armchair 2. Zigzag 3. Chiral. The stability order in these three types of CNTs are Armchair > Zigzag > Chiral [18-21]. Several kinds of Solar cells with good photovoltaic properties are being developed now days using Carbon Nanotubes. We have used the Plasma Enhanced Chemical Vapor Deposition (PECVD) process for growing the CNTs [22-26]. In earlier work peoples have used CNTs in the Solar cell but they did not give any mathematical expression for the efficiency calculation of CNT based Solar cell which is depends upon Plasma variables/parameters. In the present work, we have grown the CNTs from PECVD process and used it in absorber layer of the CNTs based Solar cell in simulation and also estimate a mathematical formula for computing Solar cell efficiency based on CNTs which is the function of various Plasma parameters like electron and ion temperature and densities. After uses of CNTs in the Solar cell we have seen an increment in the efficiency of ITO/CdS/CNTs based Solar cell up to 23-24%, which matches with the simulated and past research results almost [10]. For simulation work, we have used here SCAPS-1D software for Formation of Solar cell and computation of their efficiency. In the simulation setup, we have used the CNTs in the absorber layer and we also vary the thickness of absorber layer up to 100 to 1000 nm and noted the Solar cell related results like FF, V_{OC}, J_{SC}, efficiency, band gap etc., and after simulation we have calculated the efficiency of the Solar cell from our estimated expression and the results are very close to the value of the simulated efficiency can be seen in Fig. 11.0 and these results can be verified from many previously done researches in the past [26-29, 57-74].

2.3 SIMULATION WORK AND MATHEMATICAL MODELLING PROPOSED ON ITO, CdS, and CNTs BASED SOLAR CELL STRUCTURE

2.3.1 Simulation of ITO, CdS, and CNTs used Solar cell

2.3.1a Solar cell simulation and implement of CNTs in Solar cell

Here, we are using SCAPS-1D 3.3.10 software for ITO/CdS/CNTs based Solar cell simulation work. In Fig 1.0 CdS is illustrated in the schematic figure of the Solar cell acting as a layer of buffer between the CNT absorber layer and the ITO window layer with dimensions of (0.441 cm) x (0.440 cm) x (202 to 1102 nm) as given in Fig 1.0 and Fig 2.0. These fundamental components allow one to determine the electrical and photoelectric characteristics of a photovoltaic Solar cell. In the proposed Solar cell, the ITO and absorber layers are connected with Bi and Au material as electrical contacts [25-29].

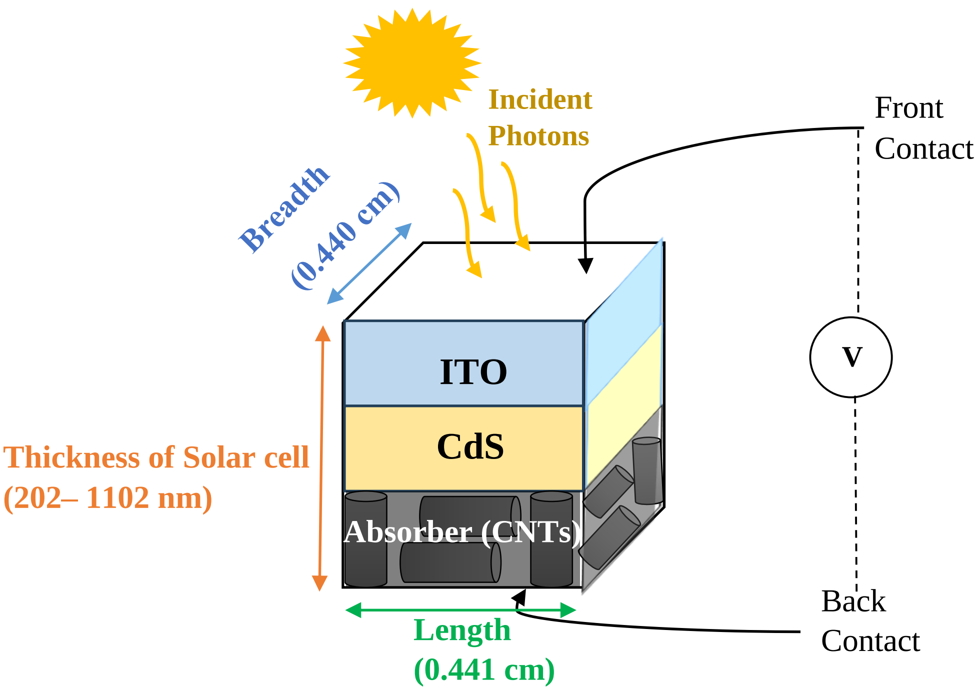


Fig. 1.0 Schematic diagram of ITO/CdS/CNTs based Solar cell

The SCAPS-1D 3.3.10 software, which was developed by the University of Gent, Belgium [30] can analyse the current density, band gap, thickness of different layers, quantum efficiency, fill factor, dark saturation current, etc. of the Solar cell. Fig 2.0 is a structure of the constructed Solar cell and captured from SCAPS-1D simulation software, in which sunlight (incident photons) falls from the side of the right contact (front) (Bi) to the left contact (back) (Au).

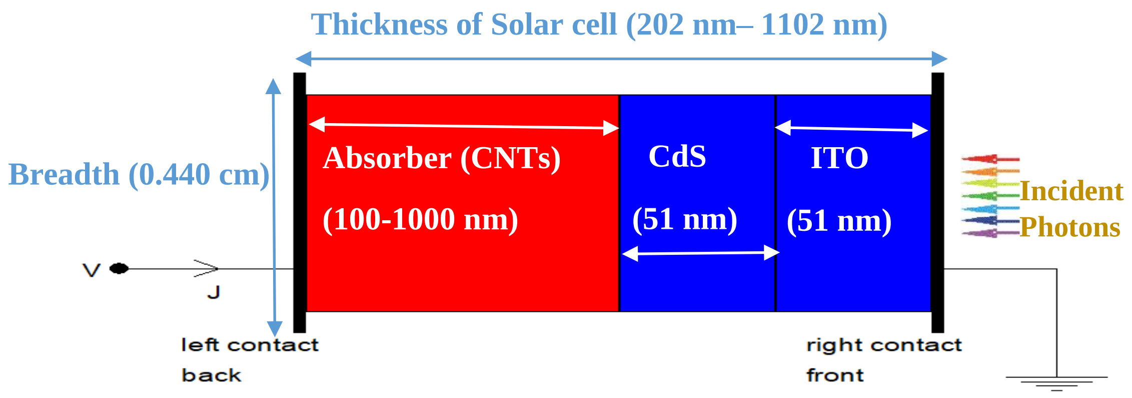


Fig. 2.0 Schematic diagram of Solar cell constructed in SCAPS-1D software

SCAPS-1D uses some basic concepts of Physics and Mathematics for semiconductor devices expressed in equations (a-c), which are as follows [25,31];

Poisson's Equation;

$$\mathrm{div}(\varepsilon.\nabla\Psi) = -\rho \tag{a}$$

We know that the continuity equation for electron carriers,

$$\frac{\partial n}{\partial t} = \frac{1}{q}\mathrm{div}(J_n) + G_n - R_n \tag{b}$$

And the continuity equation for hole carriers,

$$\frac{\partial p}{\partial t} = \frac{1}{q}\mathrm{div}(J_p) + G_p - R_p \tag{c}$$

In the SCAPS-1D simulation software, we have assumed air mass spectrum AM 1.5 of the radiation, working temperature is 300 K and an ideal condition of Solar irradiance 1 KWm^{-2} falling on the Earth and applied voltage 0.77 V in the working point section. The values of the Shunt and Series resistances are 5.0 $x10^{10}$ $\Omega.cm^2$ and 0.44 $\Omega.cm^2$, taken respectively [9,10]. The frequency of incident light is $1x10^6$ Hz taken.

Table 2 Simulation values of the proposed Solar cell layers for SCAPS -1D software [25-29];

S.N.	**Parameters**	**ITO**	**CdS**	**Absorber**
1	Layer thickness (µm)	0.051	0.051	0.1-1
2	Shallow uniform acceptor density NA (cm^{-3})	-	-	1.1×10^{17}
3	Electron mobility ($cm^2.V.s^{-1}$)	51	170	8.1×10^4
4	Layer electron affinities (eV)	4.5	4.2	4.28
5	Layer Relative dielectric permittivity	8.8	8.72	3.5
6	Electron thermal velocity in the layer ($cm.s^{-1}$)	1.1×10^7	1.1×10^7	1.1×10^7
7	Layer density of defects (cm^{-3})	-	1.0×10^{17}	1.0×10^{14}
8	Layer Band gap (eV)	3.5	2.3	1.2

9	Hole thermal velocity in the layer (cm.s^{-1})	1.1 ×10^{7}	1.1 ×10^{7}	1.1 ×10^{7}
10	In VB layer, Effective density of states (cm^{-3})	1.9 ×10^{19}	1.9 ×10^{19}	6.1 ×10^{17}
11	Hole movement within the layer (cm^{2}.V.s^{-1})	11	16	2.1 ×10^{3}
12	Shallow uniform donor density ND (cm^{-3})	1.1 ×10^{21}	1.1 ×10^{17}	-
13	In CB layer, Effective density of states (cm^{-3})	2.3 ×10^{18}	2.3 ×10^{18}	5.1 ×10^{16}

For Front and Back contact metal properties;

Table 3 Proposed Solar cell of SCAPS -1D software Metal contacts parameters [25,32-34];

S.N.	Parameters	Right contact (front)	Left contact (back)
1	Electron surface recombination velocity (cm.s^{-1})	1.0 x 10^{7}	1.0 x 10^{7}
2	Work function of used Metal (eV)	4.34	5.42
3	Hole surface recombination velocity (cm.s^{-1})	1.0 x 10^{7}	1.0 x 10^{7}

Table 4 Defect in Solar cell layers [25];

S.N.	Parameters	Absorber	ITO
1	Holes, capture cross-section (cm²)	10^{-15}	10^{-15}
2	Reference for defect energy level Et	Above EV (SCAPS<2.7)	Above EV (SCAPS<2.7)
3	Energetic distribution	Single type	Single type
4	Defect nature	Neutral	Neutral
5	Electrons, capture cross-section (cm²)	10^{-15}	10^{-15}
6	Energy level relative to the Reference (eV)	0.600	0.600
7	Nt total (cm^{-3})	10^{14}	10^{14}

2.3.2 Results regarding the simulation and discussion

Now, after putting data from tables (2, 3 & 4) in SCAPS-1D software we have obtained the results in Fig.3.0-6.0 are as follows;

2.3.2a Band gap explanation

Band gap of the constructed Solar cell in the SCAPS -1D Simulation software is as follows;

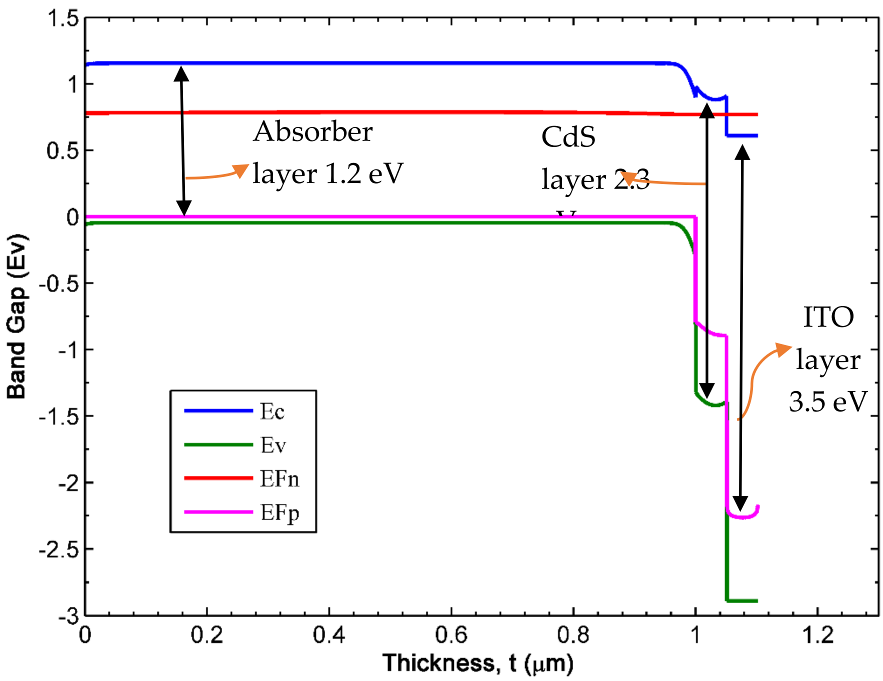


Fig. 3.0 Energy Band gap relation to thickness of the absorber layer (t) of the proposed Solar cell

Fig. 3.0 An illustration of the energy levels of various layers of a Solar cell is the energy band diagram. Fig. 3.0 illustrates the energy band diagram of the Solar cell derived from SCAPS-1D for performance analysis of the device. Since, the absorber layer made of CNTs and we know that when we increase the value of the radius of the CNTs then energy band gap will decrease, that can be seen clearly in the Fig. 3.0 [55]. To understand this band gap and radius of CNT relation, here comes a basic concept of Quantum Mechanics called Quantum Confinement. Quantum confinement processes cause the band gap of nanoparticles to grow with decreasing size. The continuous energy bands control the band structure and electronic characteristics of larger bulk materials. However, the band gap increases when a material decreases to the nanoscale because separate energy levels are formed by the confinement of electrons and holes in a very small volume. This phenomenon is understood by the idea of quantum confinement, which results from charge carriers being confined in a volume equal to their wavelength. Energy levels can be quantified when the spatial confinement of electrons and holes increases with decreasing nanoparticle size. The energy difference between the valence and conduction bands increases as a result of this quantization of energy levels.

2.3.2b The examined structures of QE curve plot, generated current density and generation and recombination plots

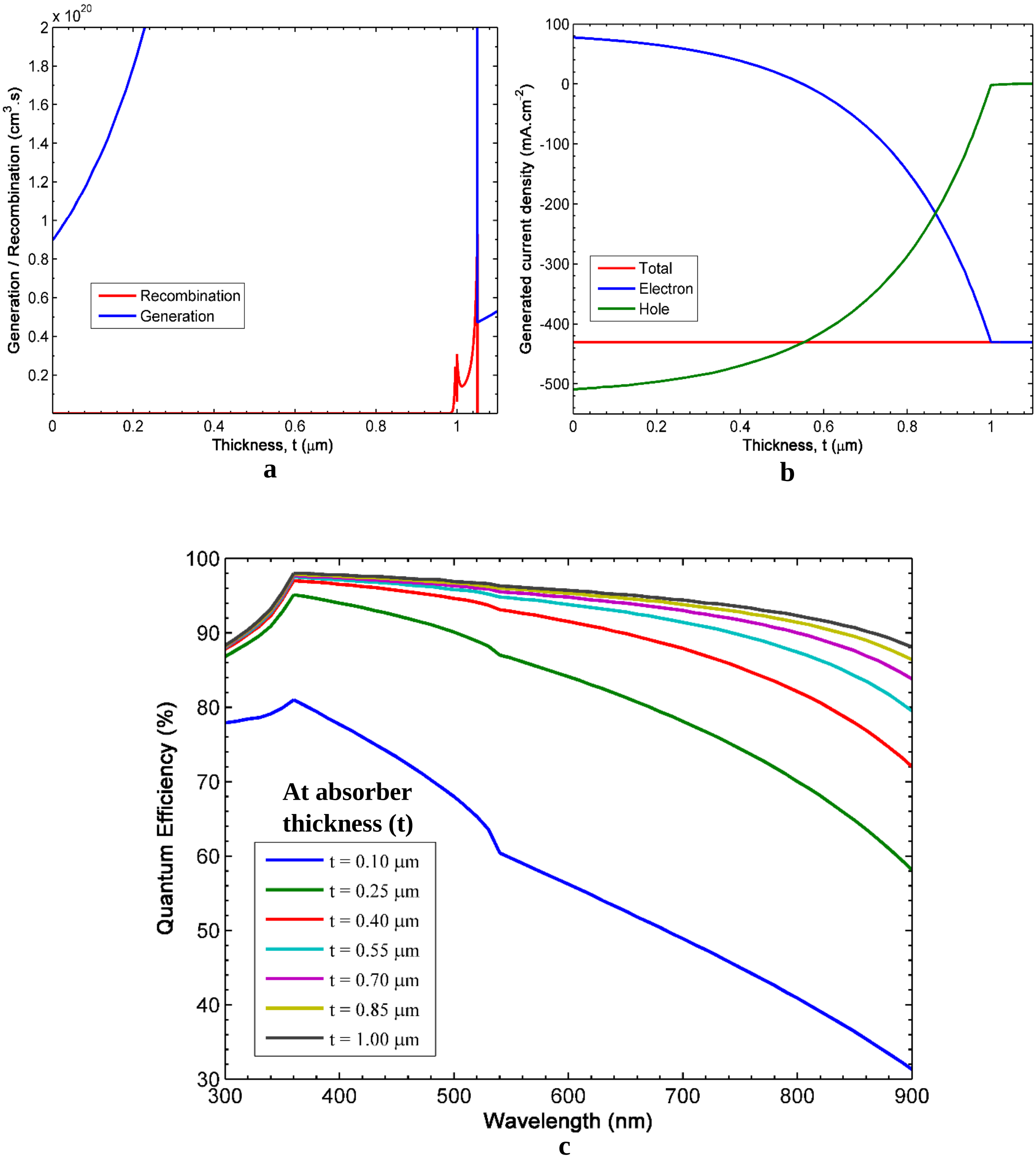


Fig. 4.0 a, b & c Generation /recombination of carriers, generated current density and QE of the SCAPS-1D simulated Solar cell. **a** Recombination and generation of carriers in relation with absorber layer thickness (t). **b** Generated current density with relation to t. **c** QE of the proposed simulated Solar cell of the incident photons with various wavelengths at varying value of t.

When sunlight falls on a semiconductor, then the electrons and holes generation and recombination take place inside the semiconductor [35-54]. Since the absorber layer consists of CNTs and they are electrically close to semiconductors then same phenomena of generation and recombination take place during this light incident process on the Solar cell. The recombination and generation with respect to the width of the absorption layer can be seen in **a** and due to this process, the charge carriers holes and electrons start moving which causes the generation of current [35-54] and that can be seen in **b** similarly, we can see the quantum efficiency of the device with respect to various wavelengths of the light in **c**, QE is decreasing with increasing value of wavelength because greater wavelength of photons have less energy, which provide less generation and recombination of carriers.

2.3.2c J-V characteristics of Solar cell at different widths of absorption layer

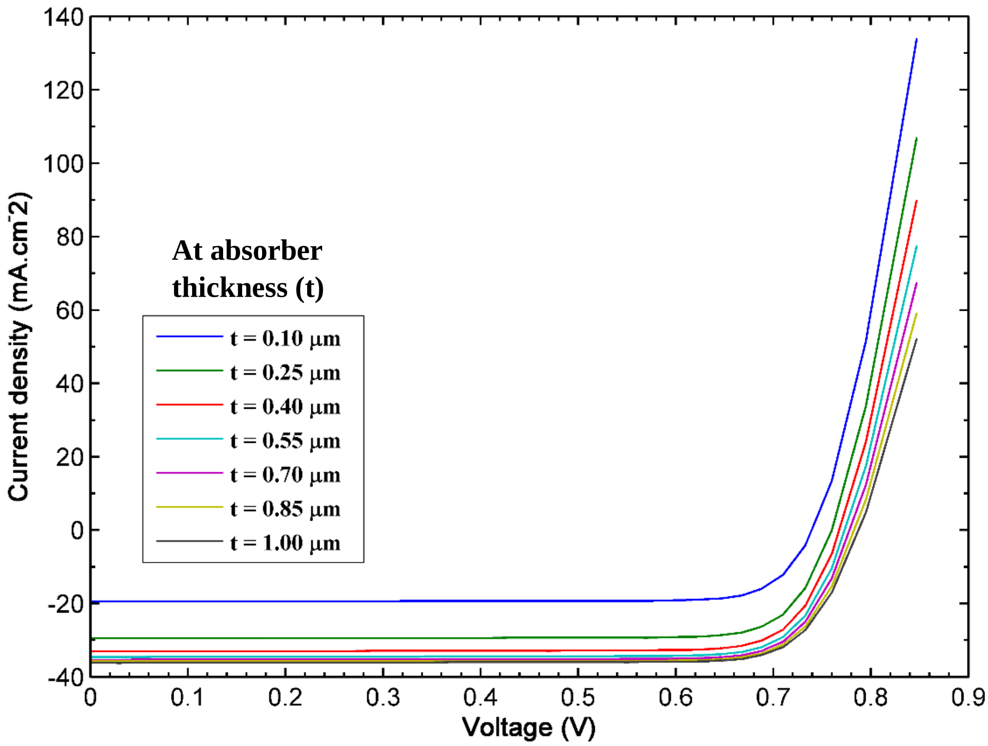


Fig. 5.0 J-V characteristic of simulated Solar cell at absorber thickness (t) of range 0.1-1.0 µm

Since, we know that for Solar cell, power generated by the cell is -(V x I) and power consumed by the cell is +(V x I). The photovoltaic process starts when the cell is exposed to the Sun at AM of 1.5. The absorption of light creates charge carriers i.e., creation of free electrons and holes in the absorption layer, which produces a continuous photocurrent [25]. Since, CNTs have very high current flowing properties or very low resistance they also have many better electrical properties like conduction, mobility, etc. which increase the current generation, leads in enhancing the efficiency of the device. In Fig. 5.0 increased thickness of the absorption layer enhances the photocurrent generated by the constructed Solar cell, which indicates that as the Solar cell's power output rises so its efficiency will also rise. Here we have taken the thickness range of the absorber layer from 100 nm to 1000 nm, which gives the efficiency of Solar cell up to 12 to 27% and it can be verified by previously done research based on the efficiency of Solar cell [10,33-34].

2.3.2d Simulated Solar cell in SCAPS-1D in relation with absorber layer thickness (t)

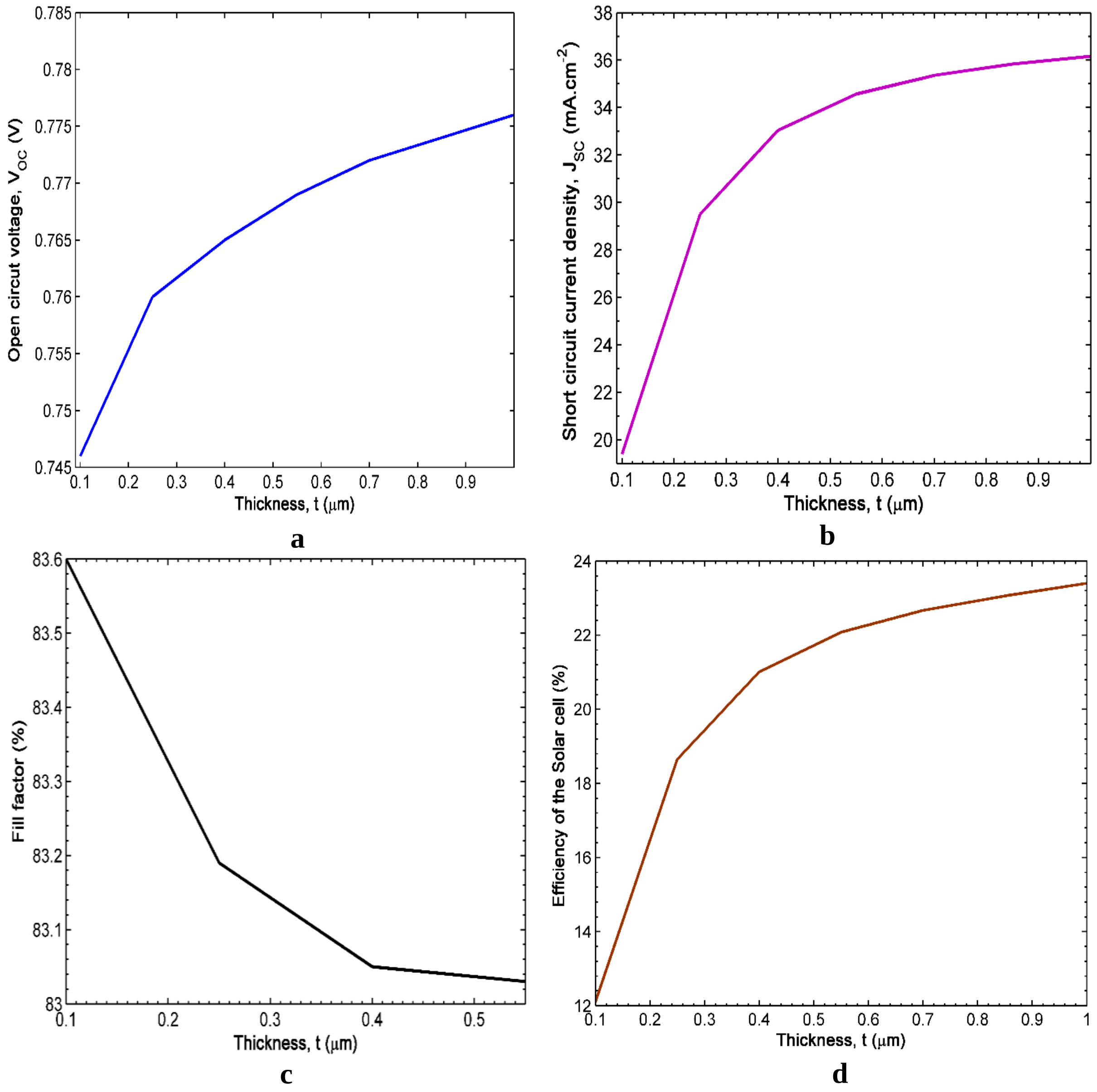


Fig. 6.0 a, b, c & d Efficiency variables of the simulated structure of the Solar cell in SCAPS-1D in relation with the thickness of the absorber layer (t). **a** Solar cell V_{OC} as relation with t. **b** Solar cell J_{SC} in relation with t. **c** Solar cell FF in relation with t. **d** Efficiency of the proposed Solar cell related to t.

In Fig. 6.0a, b & d since, in the simulated ITO/CdS/CNTs Solar cell, the absorber layer is filled with lots of CNTs so the increase in recombination and generation that happens when the absorber layer (t) thickness increases, and due to the increment in current generation that results enhancement in the efficiency of the constructed Solar cell. In Fig. 6.0**c** The parameter FF is decreasing due to the larger generation and recombination of carriers we have the larger values of J_{SC}, V_{OC}. Since, J_{SC} and V_{OC} are inversely proportional to FF [10] so, the value of fill factor (FF) is decreasing. If we explain this phenomenon from theoretical view then since we know that A Solar cell is a PN junction device which works on a basic Physics principle named as Photovoltaic effect, in this effect Carriers generations and creation occurs which leads in generation of Electric current and the special optical characteristics of Carbon Nanotubes (CNTs) allow it to absorb a wide range of light, including visible and near-infrared wavelengths. Increased absorption of sunlight by CNTs in the absorber layer of a Solar cell results in increased creation of electron-hole pairs or also called exciton, since CNTs have high charge carrier mobility property and the current loss is also decreases which results high J_{sc} and V_{oc} values. So due to the large values of J_{sc} and V_{oc} we have decrement in the value of FF of the Solar cell.

2.3.3 Summarized results from SCAPS-1D simulation

The results obtained from simulation are in table 5 as follows;

Table 5 Summary of the results from SCAPS-1D of the constructed Solar cell

S.N.	**Thickness of absorber layer (t) (µm)**	**Volume of absorber Layer (cm^3)**	**Total Thickness of Solar cell (µm)**	**FF (%)**	**V_{OC} (V)**	**J_{SC} ($mA.cm^{-2}$)**	**η (%)**
1	0.10	1.94×10^{-8}	0.202	83.60	0.746	19.406	12.10
2	0.25	4.85×10^{-8}	0.325	83.19	0.760	29.507	18.65
3	0.40	7.76×10^{-8}	0.502	83.05	0.765	33.049	21.01
4	0.55	10.6×10^{-8}	0.652	83.03	0.769	34.571	22.08
5	0.70	13.5×10^{-8}	0.802	83.06	0.772	35.359	22.67
6	0.85	16.4×10^{-8}	0.952	83.11	0.774	35.835	23.06
7	1.00	19.0×10^{-8}	1.102	83.35	0.776	36.161	23.40

2.3.4 ANALYTICAL MODELLING OF ITO, CdS and CNTs BASED SOLAR CELL

Since, we know that [9,10] the

$$\text{Efficiency of Solar Cell} = \frac{\text{Power Output } (P_{out})}{\text{Power Input } (P_{in})}$$

Solar cell efficiency (η) can be expressed mathematically as [9,10]

$$\eta = \frac{FF \times V_{OC} \times J_{SC}}{P_{in}} \times 100 \quad (1)$$

Since, photocurrent density of Solar cell is defined as [10]

$$J_{SC} = J_O \left\{ \exp\left(\frac{q(V_{OC} - JAR_S)}{n_o K_B T} \right) - 1 \right\} + \left(\frac{V_{OC} - JAR_S}{AR_{SH}} \right) - J \quad (2)$$

Now placing the J_{SC} from Eq. (2) to Eq. (1), we obtain

$$\eta = \left(\frac{FF \times V_{OC}}{P_{in}} \right) \left[J_O \left\{ \exp\left(\frac{q(V_{OC} - JAR_S)}{n_o K_B T} \right) - 1 \right\} + \left(\frac{V_{OC} - JAR_S}{AR_{SH}} \right) - J \right] \times 100 \quad (3)$$

and Power output will be

$$P_{out} = (FF \times V_{OC}) \left[J_O \left\{ \exp\left(\frac{q(V_{OC} - JAR_S)}{n_o K_B T} \right) - 1 \right\} + \left(\frac{V_{OC} - JAR_S}{AR_{SH}} \right) - J \right] \quad (4)$$

Here we are assuming that the Solar cell front face is a rectangular structure, given in Fig 1.0 so;

Area of the proposed Solar cell = Side Length × Side Width (Due to rectangular structure)

So, the expression for the area of Solar cell expressed as;

$$A = N \times (2R) \times L \quad (5)$$

Here, N is the available number of CNTs within the absorber layer, CNT radius and length are denoted by R and L.

Since, we have used CNTs in the Solar cell as absorber layer and the volume of this layer will vary with respect to CNT radius (R), length (L) and number of CNTs (N) or the only quantity that will change, is the number of CNTs when we alter the value of t maintaining the length and radius of CNT is constant. Similar to Fig. 7.0 the absorber's length and width are 0.440 and 0.441 cm, taken respectively, and its thickness (t) varies from 100 to 1000 nm.

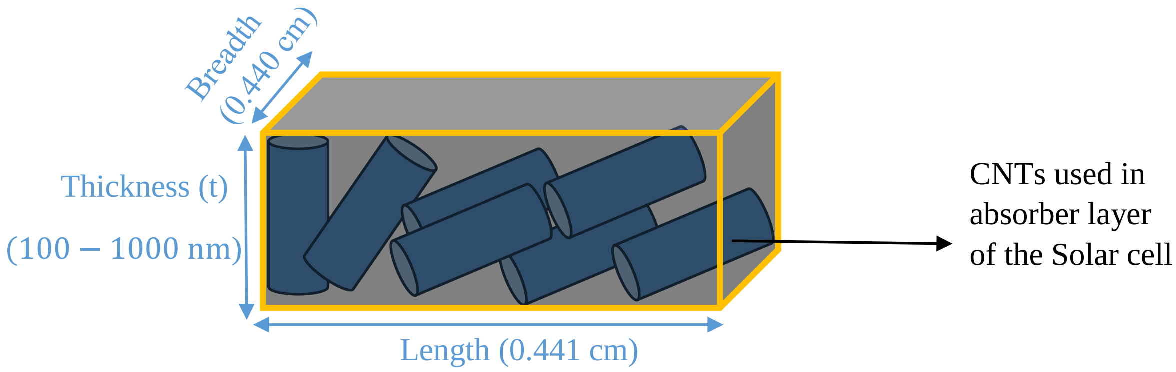


Fig. 7.0 CNTs utilized in Solar cell absorber layer

For calculating the number of CNTs (N), we use the equal volume concept i.e., the volume of the absorber layer is equal to the multiplication of the available number of CNTs and the volume of single CNT, as follows;

$$\text{Volume of absorber layer} = \text{N} \times \text{volume of single CNT}$$

Since, CNTs are a cylindrical structure so the Volume of single CNT will be $= (\pi \times R^2 \times L)$

And, Volume of absorber layer will be = Length × Breadth × Thickness of absorber layer

So

$$N = \frac{\text{Volume of the absorber layer}}{\text{Volume of single CNT}}$$

$$N = \frac{\text{Length} \times \text{Breadth} \times \text{Thickness of the absorber layer}}{\pi \times R^2 \times L}$$

Now from Eq. (5) putting the value of A in Eqs. (3) and (4), we get

$$\eta = \left(\frac{FF \times V_{OC}}{P_{in}}\right)\left[\begin{matrix} J_O\left\{\exp\left(\frac{q(V_{OC} - NL(2R)JR_S)}{n_o K_B T}\right) - 1\right\} + \\ \left(\frac{V_{OC} - NL(2R)JR_S}{NL(2R)R_{SH}}\right) - J \end{matrix}\right] \times 100 \tag{6}$$

and Power output will be

$$P_{out} = (FF \times V_{OC})\left[J_O\left\{\exp\left(\frac{q(V_{OC} - NL(2R)JR_S)}{n_o K_B T}\right) - 1\right\} + \left(\frac{V_{OC} - NL(2R)JR_S}{NL(2R)R_{SH}}\right) - J\right] \quad (7)$$

We know that the expression of radius of CNTs in terms of Plasma parameters [55-56];

$$R^2 = \exp\left(\frac{V_S L}{q}\right)\left[\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}\right]$$

or

$$R = \exp\left(\frac{V_S L}{2q}\right)\left[\sqrt{\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}}\right] \quad (8)$$

Now putting the value of R from Eqs. (8) to Eqs. (6) and (7) we get;

$$\eta = \left(\frac{FF \times V_{OC}}{P_{in}}\right)\left[J_O\left\{\exp\left(\frac{q\left(V_{OC} - 2NL\exp\left(\frac{V_S L}{2q}\right)\left[\sqrt{\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}}\right]JR_S\right)}{n_o K_B T}\right) - 1\right\} + \left(\frac{V_{OC} - 2NL\exp\left(\frac{V_S L}{2q}\right)\left[\sqrt{\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}}\right]JR_S}{2NL\exp\left(\frac{V_S L}{2q}\right)\left[\sqrt{\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}}\right]R_{SH}}\right) - J\right] \times 100 \quad (9)$$

and

$$P_{out} = (FF \times Voc)\left[J_O \left\{ \exp\left(\frac{q\left(V_{OC} - 2LN\exp\left(\frac{V_S L}{2q}\right)\left[\sqrt{\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}}\right] JR_S \right)}{n_o K_B T} \right) - 1 \right\} + \left(\frac{V_{OC} - 2LN\exp\left(\frac{V_S L}{2q}\right)\left[\sqrt{\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}}\right] JR_S}{2NL\exp\left(\frac{V_S L}{2q}\right)\left[\sqrt{\frac{1}{4\pi q^2\left(\frac{n_{eo}}{T_{eo}} + \frac{n_{io}}{T_{io}}\right)}}\right] R_{SH}} \right) - J \right] \quad (10)$$

2.3.5 ANALYTICAL RESULTS

Since, we have done our work in two parts first is, to fabricate CNTs by using the PECVD method, and second is, to use these CNTs in the Solar cell absorber layer. For analytical calculation, we will use the V_{OC}, J_{SC}, J_o, n_o, R_S, R_{SH} and P_{in} values at different thickness of the absorber layer, which have been obtained from the SCAPS-1D simulation which is summarized in table 5. For mathematical calculation and results we use some constant values that are taken from the SCAPS 1-D simulation setup, which are given in table 6.

Table 6 Constant values for mathematical calculation

S.N.	Parameter	Value
1	P_{in}	1000 $W.m^{-2}$
2	q	1.6 x 10^{-19} C
3	R_S	0.44 $\Omega.cm^2$
4	R_{Sh}	5.0 x 10^{10} $\Omega.cm^2$
5	K_b	1.38 x 10^{-23} $j.K^{-1}$
6	T	300 K
7	n_o	2.1

2.3.5a Solar cell efficiency in relation with Plasma parameters (n_{eo}, n_{io}, T_{eo}, and T_{io})

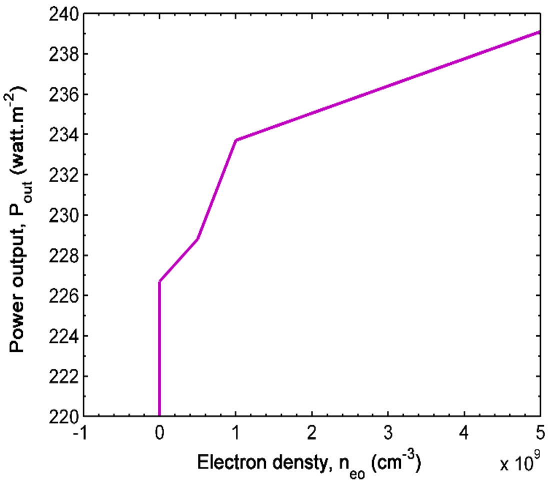
To know the effects of Plasma parameters on the efficiency of Solar cell analytically, we will take the required PECVD data from table 7 in the work (1) section [55-56] and also from table

6 which are essential for solving the Eqs. (6), (7) and (9) to get the value of the efficiency of Solar cell. When we put the all-parameter values in Eqs. (9) and (10), we get the solar cell's power output and efficiency which are given in table 7 in the work (2) section.

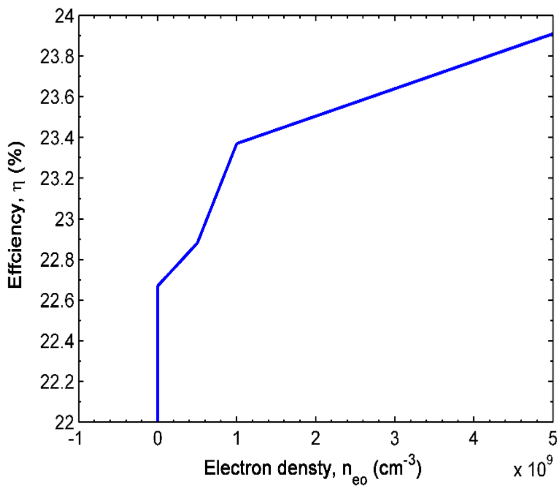
Table 7 Calculated efficiency of Solar cell from Eqs. (6), (7) and (9), we get

Work (1) Results from PECVD method							**Work (2) Results from simulation and analytical work**						
S. N.	**n_{eo} (cm^{-3})**	**n_{io} (cm^{-3})**	**T_{eo} (K)**	**T_{io} (K)**	**R (nm)**	**L (µm)**	**t (µm)**	**N**	**V_{OC} (v)**	**FF (%)**	**J ($mA.cm^{-2}$)**	**J_O ($mA.cm^{-2}$)**	**η (%)**
1	1.0×10^{7}	5.0×10^{6}	5800	2400	2.0	0.1	0.10	1.5×10^{12}	0.746	83.60	18.59	0.45×10^{-4}	12.42
2	5.0×10^{6}	4.2×10^{6}	5220	2300	3.0	0.1	0.25	1.7×10^{12}	0.760	83.19	28.22	0.49×10^{-4}	18.89
3	1.0×10^{6}	2.5×10^{6}	4640	2200	4.0	0.1	0.40	1.5×10^{12}	0.765	83.05	31.63	0.50×10^{-4}	21.22
4	1.0×10^{5}	1.0×10^{6}	3480	2100	5.0	0.1	0.55	1.3×10^{12}	0.769	83.03	33.09	0.49×10^{-4}	22.67
5	5.0×10^{8}	5.0×10^{7}	12760	2180	5.0	1.0	0.70	1.7×10^{11}	0.772	83.06	33.83	0.47×10^{-4}	22.88
6	1.0×10^{9}	5.0×10^{8}	13920	2210	5.0	2.0	0.85	1.0×10^{11}	0.774	83.11	34.26	0.46×10^{-4}	23.37
7	5.0×10^{9}	1.0×10^{9}	15080	2250	5.0	3.0	1.00	8.2×10^{10}	0.776	83.35	34.66	0.45×10^{-4}	23.91

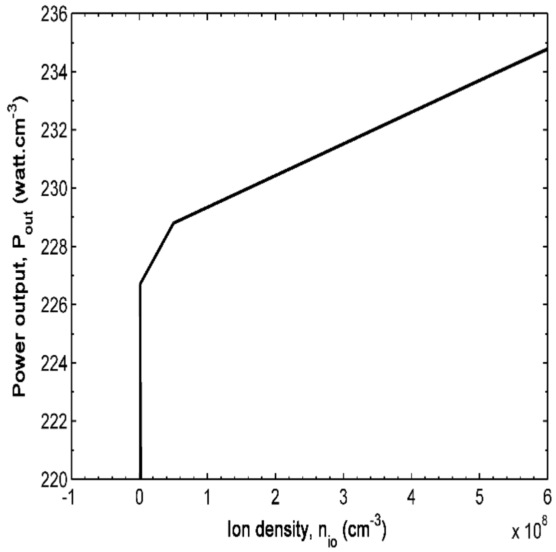
2.3.5b Influence of Plasma parameters electron and ion densities (n_{eo} and n_{io}) on Solar cell



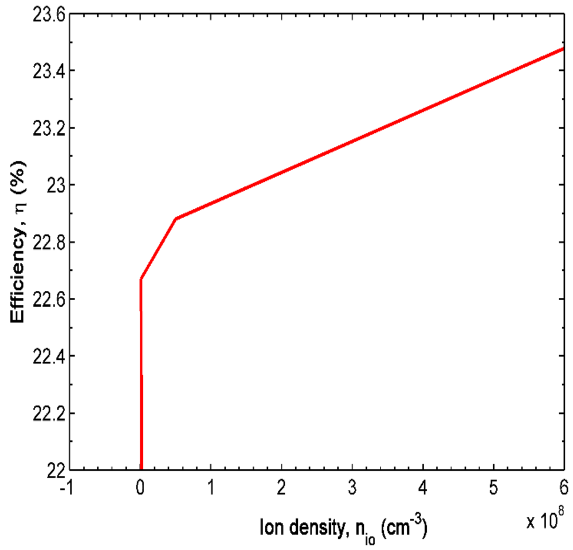
a



b



c



d

Fig. 8.0 Solar cell efficiency and power output in relation to Plasma parameters electron and ion density (n_{eo} and n_{io}). **a** Power output of the Solar cell with relation to electron density (n_{eo}). **b** The Solar cell efficiency with respect to electron density (n_{eo}). **c** Power output of the Solar cell in relation with ion density (n_{io}). **d** Solar cell efficiency with respect to ion density (n_{io}).

In Fig. 8.0,we have Solar cell power output and efficiency corresponding to electron and ion densities (n_{eo} and n_{io}). In Fig. 8.0a-d, we see that when we raise the values of the electron and ion density Plasma parameters (n_{eo} and n_{io}), the output power of the proposed Solar cell is increasing. The reason behind that is we know that when we increase the same Plasma parameters n_{eo} and n_{io} then the radius of CNTs will decreases, which leads to an increase in the voltage output of the device [55-56], and due to the increasing value of voltage, leads an increment in the power output and efficiency of the Solar cell. To understand this phenomenon, the increased electron density (neo) and ion density (nio) parameters in PECVD process typically result in a larger concentration of reactive species and energy in the plasma. The deposited Carbon Nanotubes create and growth dynamics may be influenced by this higher energy and reactivity. Because higher plasma densities and input power can encourage more quickly nucleation and growth rates of carbon nanotubes, so the radius of the CNT decreases with increasing plasma parameters. CNT radius may decrease as a result of this faster growth and producing thinner CNTs. Furthermore, the etching effect in which reactive species in the plasma may degrade the CNTs sidewalls during growth can be improved by raising plasma parameters. Thinner tubes can be obtained by this etching action which contributes to decreasing the CNT radius. At the interface between the CNTs and the active material (e.g., buffer layer, ITO), smaller diameter CNTs could provide a stronger electric field. A higher voltage output may result from this facilitating more effective separation of photogenerated electron-hole pairs. Moreover, smaller CNTs can provide a more direct route for charge carriers to reach the electrode, hence lowering recombination losses and raising charge collecting efficiency. This may result in a greater current, which, by Ohm's law, might raise the voltage output because of changes carried on by the plasma treatment, the effective surface area of the CNTs could increase while the radius decreases. Due to this more active region for charge generation and photon absorption we have higher current and voltage production.

2.3.5c Effect of electron and ion temperatures (T_{eo} and T_{io}) on Solar cell

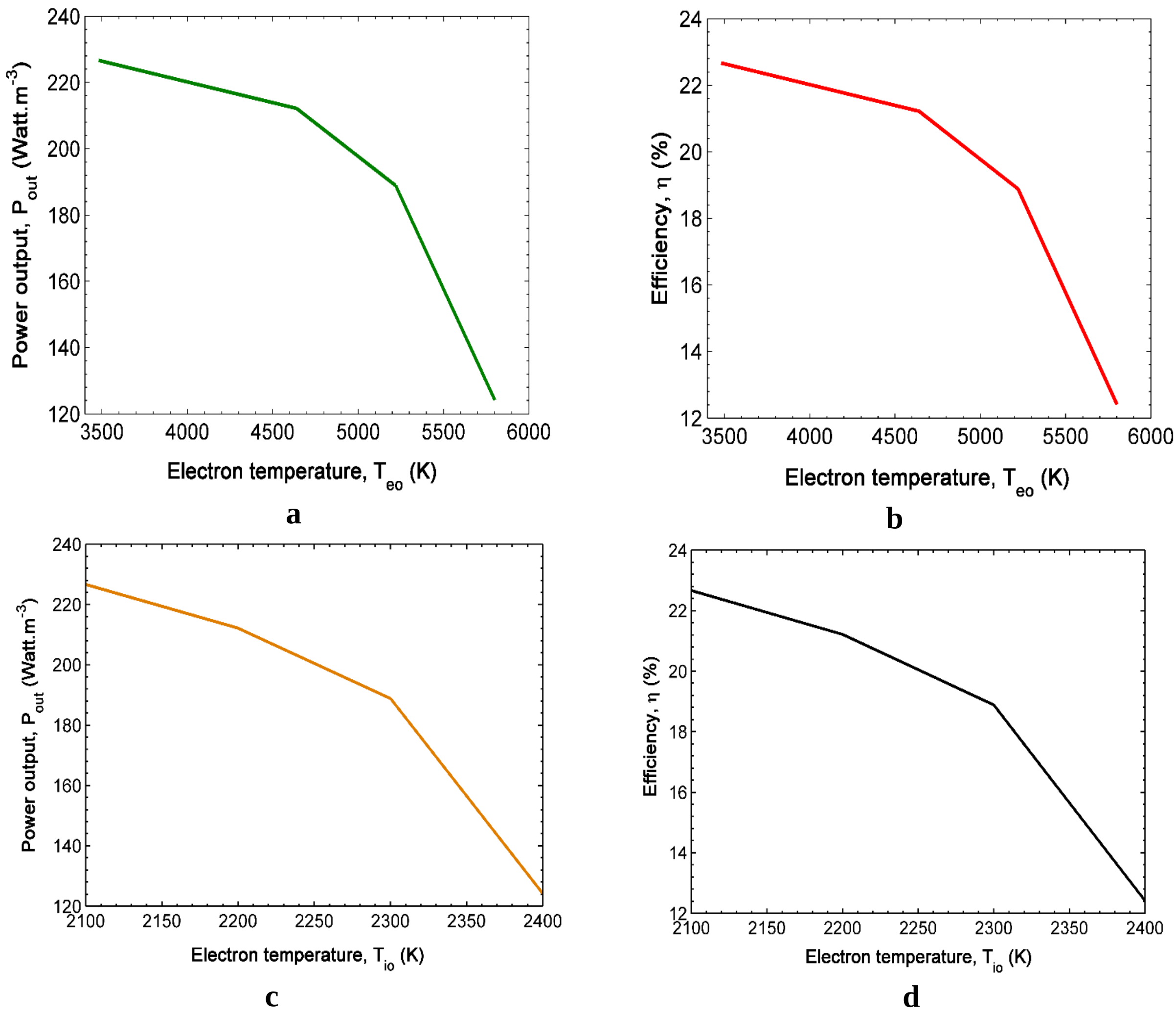
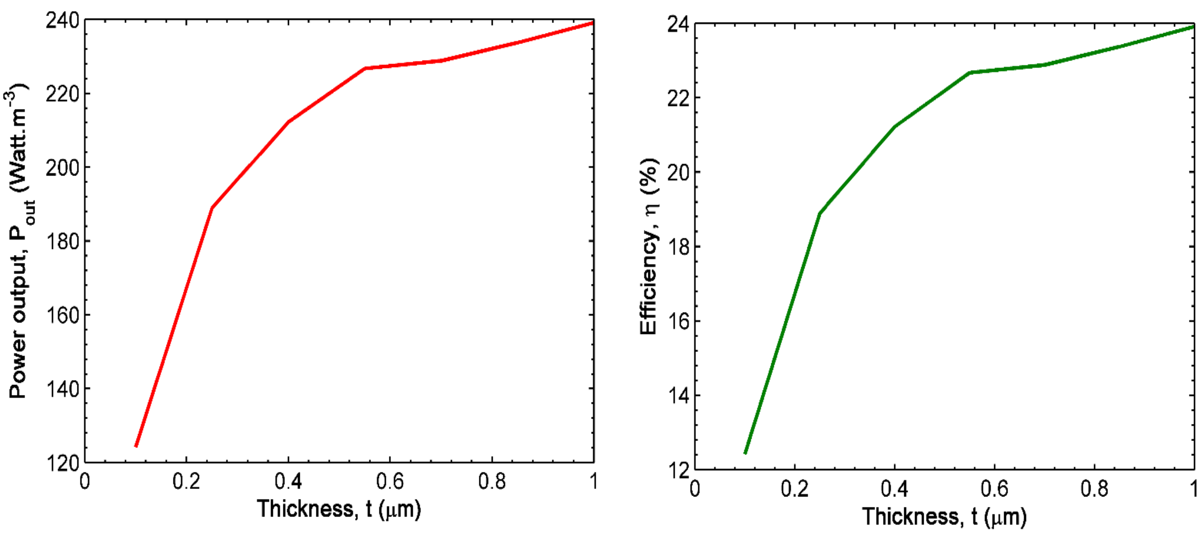


Fig. 9.0 Solar cell efficiency and power output in relation to Plasma parameters electron and ion temperature (T_{eo} and T_{io}). **a** Solar cell output power with respect to electron temperature (T_{eo}). **b** Efficiency of the Solar cell in relation with electron temperature (T_{eo}). **c** Power output

of the Solar cell relation with ion temperature (T_{io}). **d** Efficiency of the Solar cell relation with ion temperature (T_{io}).

For Fig. 9.0, we have Solar cell power output and efficiency corresponding to electrons and ions temperature (T_{eo} and T_{io}). For Fig. 9.0a-d, when we are increasing the value of Plasma variables electron and ion temperature (T_{eo} and T_{io}) therefore the output power of the Solar cell is dropping. The reason behind that is, we know that when we increase the electron and ion temperature (T_{eo} and T_{io}) then the radius of CNTs will increase, that leads to decrement in voltage output of the device [55-56] and due to this decreasing value of voltage, that leads to decrement in power output and efficiency of the Solar cell. To understand this phenomenon, during synthesis procedures like PECVD, electron and ion temperature can affect CNT growth and stability. Faster growth rates and structural changes in the generated Carbon Nanotubes can be enhanced via higher temperature. However, the particular impact on the radius of CNTs can vary according to a number of variables, including the type of catalyst, the synthesis technique, the growth environment, and the kind of CNT (single-walled, multi-walled, etc.) being generated. As higher electron and ion temperature in PECVD process, CNTs can have bigger diameters because of faster growth kinetics and enhanced carbon diffusion. At the interface between the CNTs and the active material (e.g., buffer layer, ITO), larger diameter CNTs could provide a weaker electric field. A lower voltage output may result from this facilitating less effective separation of photogenerated electron-hole pairs. This may result in a low current, which, by Ohm's law, might decrease the voltage output. Because of changes carried on by the plasma treatment, the effective surface area of the CNTs could decreases while the radius increases. Due to this less active region for charge generation and photon absorption we have Low current and voltage production.

2.3.5d The effect of thickness of absorber layer (t) on the performance of the Solar cell



a **b**

Fig. 10.0 Power output and efficiency of ITO/CdS/CNTs based Solar cell are influenced by absorber layer thickness (t). **a** Output power of the Solar cell with respect to t. **b** Solar cell efficiency in relation to t.

In Fig. 10.0, Solar cell efficiency varies with absorber layer thickness (t). Fig. 10.0a, b when we increase the absorber layer thickness, then power output and efficiency of the Solar cell are increasing the reason behind that is, when increase the thickness of the absorber layer of the Solar cell then number of CNTs are increases and that leads to increment in output voltage that will increase the power output and efficiency of the Solar cell [55-56].

2.4 COMPARISONS OF EFFICIENCY OF THE SIMULATED AND THE ANALYTICAL MODEL OF THE PROPOSED ITO/CDS/CNT BASED SOLAR CELL

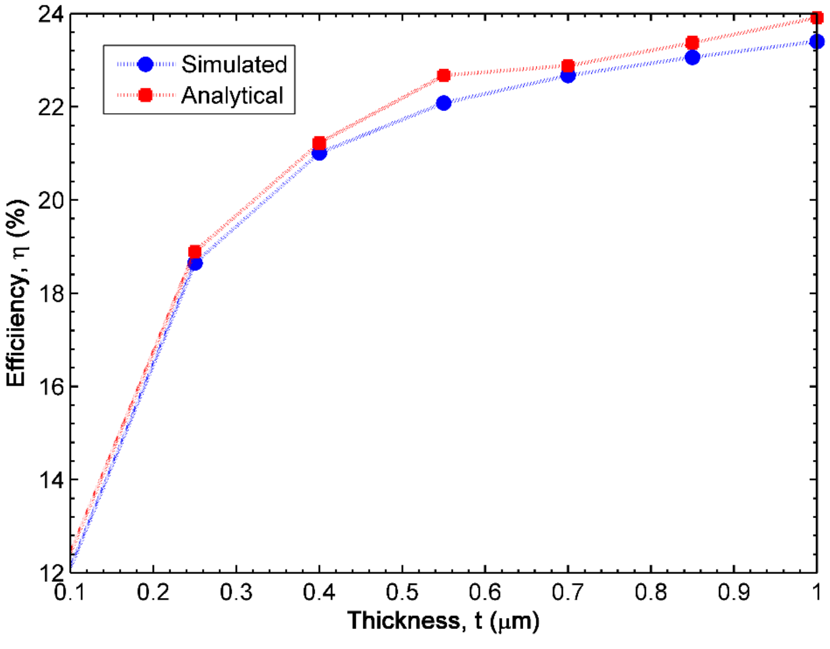


Fig. 11.0 The efficiency of the constructed Solar cell determined from analytical and simulation work.

For Fig. 11.0, this is the efficiency of the constructed Solar cell captured from simulation and analytical work is shown. In this figure, we can see that when we increase the value of t then efficiency of the Solar cell rises and the little difference between the analytical and simulation results may be because of environmental defects like operating temperature, Solar irradiance fluctuation, etc.

2.5 PERCENTAGE ERROR IN THE EFFICIENCY OF THE SOLAR CELL BETWEEN SIMULATION AND ANALYTICAL WORK

We know that the expression for the,

$$\text{Percentage error for the efficiency of the Solar cell}(\%)$$
$$= \left|\frac{\text{Simulated Value} - \text{Analytical Value}}{\text{Simulated Value}}\right| \times 100$$

Table 8 Percentage error between Simulated and Analytical results

S.N	Efficiency of the Solar cell		Error (%)	Average (%)
	Simulated Result (%)	Analytical Result (%)	$\left\lvert\frac{\text{Simulated Value} - \text{Analytical Value}}{\text{Simulated Value}}\right\rvert \times 100$	$\frac{\text{Total sum of error}}{\text{No. of total error}}$
1	12.10	12.42	2.64	$\frac{2.64 + 1.27 + 0.99 + 2.67 + 0.92 + 1.34 + 2.17}{7}$ = **1.71 %**
2	18.65	18.89	1.27	
3	21.01	21.22	0.99	
4	22.08	22.67	2.67	
5	22.67	22.88	0.92	
6	23.06	23.37	1.34	
7	23.40	23.91	2.17	

So, the Percentage error between Simulation and Analytical work is 1.71%.

2.6 SYNOPSES OF THE CURRENT WORK

Synopsis of the entire work is in table 9;

Table 9 Summary table for impact of the different factors on Solar cell efficiency

S.N.	Parameter	Parameters Effect on Solar cell efficiency
1	N_{eo}	Increases with increasing the value of n_{eo}

2	Nio	Increases with increasing the value of n_{io}
3	T_{eo}	Decreases with increasing the value of T_{eo}
4	T_{io}	Decreases with increasing the value of T_{io}
5	t	Increases with increasing value of t

2.7 CONCLUSION

The proposed Solar cell is equipped with CNTs as an electron acceptor, and those CNTs are grown using the PECVD technique. In PECVD, we have some Plasma parameters like electron and ion temperatures, densities, etc., and we investigated here the effect of Plasma characteristics (electron and ion temperatures, densities) on the Solar cell. In our work, we have done simulation work as well as theoretical modelling, and the results of both are very close. This can be seen in error calculation which is about 1.7%. Here, we adjust a number of Plasma parameters that can impact Solar cell efficiency. Since, there is no expression that can directly relate Plasma variables to the efficiency of the Solar cell, we have solved this problem in the present work and successfully established a correlation between the Solar cell efficiency and Plasma parameters. The results obtained from our work match very closely to the recent research [57-74]. CNTs implication, which provides the next step of the research, and our efficiency with respect to Plasma parameters can be a very important result in describing more research results that will be done in the future work. Here we have taken the PECVD grown CNTs in the absorber layer. For future work CNTs can also be used in HTL, ITO, ETO like layers through which Solar cell performance may be enhanced.

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