A

DISSERTATION REPORT

ON

COUPLING IMPROVEMENT IN THIN FILMS USING METAL NANOPARTICLES FOR SOLAR CELL APPLICATIONS

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MASTER OF TECHNOLOGY

in

WIRELESS AND OPTICAL COMMUNICATON

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DEPARTMENT OF ELECTRONICS AND COMMUNICATION ENGINEERING

by

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(2017PWC5427)

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JAIPUR (RAJASTHAN) – 302017

Certificate

This is to certify that the dissertation report entitled **"Coupling Improvement in Thin Films using Metal Nanoparticles for Solar Cell Applications"** submitted by **Avneesh (2017PWC5427)**, in the partial fulfilment of the Degree Master of Technology in **Wireless and Optical Communication** of Malaviya National Institute of Technology, is the work completed by him under our supervision, and approved for submission during academic session 2018-2019.

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Declaration

I, Avneesh, declare that this Dissertation titled as "**Coupling Improvement in Thin Films using Metal Nanoparticles for Solar Cell Applications**" and the work presented in it is my own and that, to the best of my knowledge and belief.

I confirm that the major portion of the report except for the referred works contains no material previously published nor present a material which is to be substantial extent has been accepted or the award of any other degree by the university or another institute of higher learning. Wherever I used data (Theories, results) from other sources, credit has been made to that source by citing them (to the best of my knowledge). Due care has been taken in writing this thesis, errors and omissions are regretted.

Date: **AVNEESH**

Place: ID: 2017PWC5427

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Abstract

The source of almost all of the earth's energy is solar energy in one form or another. For warmth and food, all living humans depend on the sun. And individuals use the energy of the sun in many other respects as well. For example, fossil fuels, crop material from an ancient geological era, are used for electricity generation and transportation, and solar energy from thousands of years ago is mainly stored. Biomass transforms energy of the sun into a eco-friendly fuel and can use for heat, transportation or electricity. Whereas wind energy also helpful in providing mechanical energy or transportation through the use of air current generated by solar's heated air and earth's rotation. Wind turbines also transform wind power into electricity. So, a device name Photovoltaic cell can also help us to convert the solar energy into electricity and can be stored to use later.

Now, these photovoltaic cell classified into 3 generations.1^{st} generations consist of a thick wafer of Silicon solar cell. In a 2^{nd} generation, thin films solar cell comes whose thickness is in the range of the few micrometres. And in the 3^{rd} generation, there are Dye-sensitized solar cell and also the Organic solar cells. 2^{nd} and 3^{rd} generation solar cell is better than the 1^{st} generation in many aspects. But they failed when it comes to the cost. As the 1^{st} generation is cheaper than the other one. Hence used widely around the world by 80 % of the people. But thin film is better than the 1^{st} generation in installation, covering less area and many more. But they show less efficiency because of the thickness of the substrate. As more light cannot trap in the substrate due to the thickness of the film.

Thus to trap the light in the thin film solar cell. Metal nanoparticles are used. And with their plasmonic effect, absorption of light can be enhanced. As due to plasmonic effect light will scatter from the nanoparticles into the active layer and its optical path length can be increased. That how absorption can be enhanced and the efficiency too.

In this thesis, thin film of Gallium Arsenide couple with the metal nanoparticles of different materials like silver, gold, copper, and aluminum. And observing the structure about how much the absorbance of light by active layer. By observing graph of reflectance and transmittance. If they show minimum value, then the light has been absorbed very well. The structure is optimized by varying the material of the NPs, by increasing their size and by arranging them at different positions. Then that optimized structure can be used for the solar cell applications.

List of Abbreviation

TIR	-	Total internal reflection
OL	-	Observation line
PW	-	Peta watts
AM	-	Air mass
DC	-	Direct current
AC	-	Alternating current
NPs	-	Nanoparticles
ARC	-	Anti-reflection coating
SPR	-	Surface plasmon resonance
LED	-	Light emitting diode
SRH	-	Shockley-read-hall-recombination
EM	-	Electromagnetic
PV	-	Photovoltaic

List of Symbols

eV	-	Electron Volt
dB	-	Decibel
µm	-	Micrometer
nm	-	Nanometer
mW	-	milliwatt
cm	-	centimeter
eJ	-	Exa joules
J	-	Joules
E	-	Energy
h	-	Planck constant
N	-	Refractive Index
λ	-	Wavelength
L	-	Length
L0	-	Path length from zenith
η	-	Efficiency
P_{max}	-	Maximum power
τ	-	Transmittance
V	-	Voltage
α	-	Absorbance
r	-	Reflectance

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Chapter 1. Introduction

1.1 Introduction

According to the 2017 report given by the United Nations, the population of the world is growing from 7 billion to 8 billion by the end of 2030. Every year approximately 80-83 million people are increasing [1]. This growing population is strongly affecting the consumption of energy by mass. The consumption of primary energy (oil, coal, natural gas, solar energy, hydroelectricity and more) increases from 1.2 percentage in 2016 to 2.2 percentage in 2017 stated by BP magazine [2]. Around 70-80 percentage of energy has been drawn out from sources like natural gas, oil, and coal. Such usage of resources can lead to scarcity in less time. But this will not happen if we use solar energy. For example, the sun is responsible for the evaporation, it takes water from the sea and refills the rivers via rain. Thus the sun is the source of hydroelectricity indirectly. So in renewable resources, solar energy is the good option nowadays and can fulfill the demand of energy for the world. Photovoltaic is a refined and easy way to utilize the sun's energy.

Our planet receives around 89 PW (petawatts) of radiation from the sun via the atmosphere at the livelihood regions of humans. Around 3,850,000 eJ of the heat per year is absorbed by the sea, lakes, clouds, and lands. This figure is larger than the consumption of energy globally. Hence it can be said that solar energy is the prime and eternal source. Therefore, to eliminate the shortage of electricity, Photovoltaic device is used for the conversion of solar energy to electricity that is in DC voltage. An inverter is installed which helps in transformation of generated Direct current into AC and can be stored in the batteries for further commercial usage.

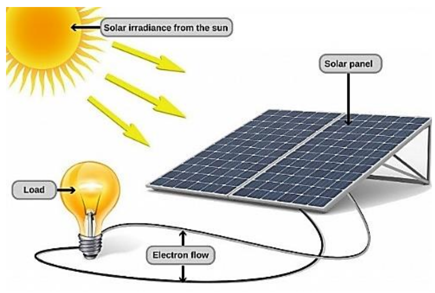


Figure 1.1 Solar irradiance from the sun [3].

Now Photovoltaic cell can be classified into 3 generations that depends on the substrate's thickness and materials used in it. Under first-generation solar cells, silicon fabricated solar cell is used. These solar panels are used around 80% of the world.it is just because of the availability of the silicon element on earth is an enormous amount just after oxygen. They are Mono-crystalline, polycrystalline and Amorphous Si cells with an efficiency of around 6%. 2nd generation solar cells consists of compounds like Cadmium Telluride, Amorphous Silicon, Copper Indium, and Gallium Arsenide. They are generally called as thin films solar cell as their thickness is less than those of first generation cells. And in 3rd generation solar cell, we have Dye-sensitized, Organic, and Perovskite solar cell [4].

1.2 Need of Solar Cells

At first, the Photovoltaic effect is the process of using solar cells directly converting sunlight into electricity. It is now the best renewable alternative approach to generating electricity from standard fossil fuels, but a comparative newcomer in relation to other approaches. In the 1950s, the first practical photovoltaic systems showed up. In 1960s, Photovoltaic's development boosted for the space sector, as there was need of distinct power supply for satellite apps from "grid" energy. But they were more costly than what they are nowadays, and apart from grid power, the need for a generation of electricity technique was quite a decade away due to improvement in silicon materials, solar cells are growing in the market. In 1970s, world faced an oil crisis that make the world‘s attention towards the need for alternative energy sources. This condition results in the advancement of photovoltaic cells as a source for producing terrestrial energy. There are a few advantages of Solar cell, which are as follow:

- **Solar energy is safe and clean.** It can replace fossil fuels and gas to produce electricity that affects the environment in a destructive way. World Wildlife Fund shows the figure that electricity produced by fossil fuels and gas results in damaged forest areas, acid rain and affect the agricultural sector. This lead to the loss of billions of dollars around the world. So the use of solar energy will eliminate this cause.
- **Prevent habitats from destruction**. Trees and forests are being destroyed for fossil fuels. So these renewable energy is a better option to use worldwide.
- **Action against drastic change in the climate.** Due to pollution and all dangerous gases, there is a rise in global temperature and abnormal change in the climate. This

leads to the heat waves and spreading of diseases among people to cause health problems.

So, solar power can stop all the adverse effect on climate by providing the eco-friendly power source and providing economic benefits to society [5].

1.3 Thesis Organisation

There are six chapters organized in this thesis including the introduction part which contains the motivation behind the project and the objective or need of the project. This is the 1st chapter which is followed by chapter 2 that contains the literature review of the project.

Chapter 3 have the fundamentals of the solar cell. From solar light of the sun to the efficiency of the photovoltaic cell, each topic is being described in full detail. This chapter gives the idea of how solar radiation is converted into light, about parameters that needed, material that to be used and the process occurs in the photovoltaic cell. At last, describing the efficiency of it.

Chapter 4 gives the idea of the basics needed for the project. Our project is related to the coupling of thin films with the nanoparticles for solar applications. So it contains about how the absorption in thin films occurs, which factors affect them. And also how to trap the light in them.

Chapter 5 contains the simulation part. First basic knowledge of materials is being used described in detail. Then discussed the dimensions of the structure which is needed for the analysis. After describing, simulation results are being analyzed. These results are the graphs obtained from the Optifdtd software of Optiwave systems. They have been compared by slightly changing the structure for optimization.

Chapter 6 consists of the conclusion of the optimized structure's results and observation of how they behave with respect to the solar spectrum and describe the future scope of that structure for solar applications.

Chapter 2. Literature Review

In 2007, Stefan A. Maier through his book on fundamentals and applications of plasmonics provide the basic knowledge about the surface plasmon polaritons at metal or insulator interfaces. It tells about the behaviour of the electromagnetic waves with regarding metals and many more and also about localized surface plasmons [21].

Yu.A. Akimov,W.S. Koh1, and K. Ostrikov analyzed high order surface plasmon modes by using predictive 3D modeling. They exhbit the enhancement of optical absorption in silicon (amorphous) solar cells by embedding silver NPs and later they suggest how to optimize the NP array parameters in 2009 [13].

In 2009, Dr. Jeffrey L. Taylor in his work shows the reflectance measurements for solar cell. They have given a basic idea about the specular reflection and also about the diffuse reflection and about the other basic concepts regarding the absorption, transmission, and reflection and also about their interrelation among each other [16].

In 2010, Gia-Wei Shu, Wei-Chuan Liao, Yueh-Chien Lee, Ja-Yuan Lee, I-Jen Hsu, Ji-Lin Shen, Ching-Ling Hsu, Min-De Yang, Chih-Hung Wu, and Wu-Ching Chou have increased the conversion efficiency of Gallium Arsenide solar cell by embedding silver NPs. They have specified the sizes of particles between the 11.4 to 17.2 nm. The achieved increment is 20.2 percentage in efficiency. They gave the reason behind this achievement is the effect of SPR and interband transition together [25].

In 2010, Harry A. Atwater and Albert Polman proposed the methods to localize light in nanoparticle via plasmonic effects. They show different designs of how to use plasmonics to yield better absorption in photovoltaic devices. Different approaches are shown for light trapping by reducing the thickness of solar cells [22].

In 2013, Razan Nejm, Ahmed Ayesh, and Mousa Hussein proposed the structures of silver NPs embedded in the silicon solar cell. They have trapped the light in the thin layer by using a single antireflection coating that is Si_3N_4 . And minimize the reflection losses at the front surface of the cell. Silver NPs gives the best results when embedded into the ARC surface compare to other placed positions. Also decreasing the refractive index plays an important role in improving solar cell behaviour [26].

In 2013, Henry A. Aribisala in his theses improved the photovoltaic power system's efficiency. He has explained the concept of solar irradiance very well. Give a brief knowledge about the different value of irradiance from the sun in a vacuum, at earth atmosphere and at the poles of the earth. He describes the concept behind the Air Mass coefficient very well [7].

In 2015, Chetan Singh Solanki's book was published, which provided the fundamentals, technologies, and applications of the solar cell. It discussed the thin film solar cell very well. Tells about the advantages and disadvantages of using it and much more [17].

In 2016 Kiran Ranabhat, Aleksandra Antal'evna Revina, Leev Patrikeev, Kirill Andrianov, Valerii Lapshinsky, and Elena Sofronova publish a review paper about the generation of the solar cell. It tells about the latest modifications occur in the data about the first, second and third generation of solar cell.it also gave an idea about the global solar market, cost of the solar panel at present day. They also discuss the future idea of implementing the panels on cars and free them from gas and diesel [4].

In 2016, Gurjit Singh and Verma SS have designed thin films with the different geometries and materials of nanostructures. Excitation of nanoparticles on their surface plasmon resonance and increase the efficiency to around 8 percentage. They give the basic idea of the localized surface plasmon resonance (LSPR) and also about the scattering of light by metal NPs [12].

In 2017, Ibrahim Khan, Khalid Saeed and Idrees Khan provided a detailed overview of the nanoparticles basics that are synthesis, properties and the applications of different forms of nanoparticles. They classified them into different categories. Whether it would be metal NPs or ceramic NPs. They show which NP imparts which colors due to absorption in the visible region [23].

In 2017, Nipon Deka, Prashant K. Saraswat, Gagan Kumar, and Maidul Islam analyzed the performance of device having double nanoparticle system on the substrate of silicon. The factors which affect them is the distribution of these NPs in space and their relative position with each other. With the presence of double nanoparticle system, there is an enhancement of photon's coupling into the plasmonic modes and increase the absorption of the photons over a wide range [28].

In 2017, Dezhong Zhang and Yang Tang enhance the reflective properties of ITO by the effects of plasmons by silver NPs. We study the effect of size of the particle and distance among them on reflection increment. It also tells about the transmittance of light through the silver NPs decreases with the increase in the size metal NPs. which is explained by the Mie theory [27].

Neha Singh, Ravindra Singh Chauhan, and Pawan Kumar Inaniya in 2017 increase the trapping of light that minimizing the reflections and enhance the AR property of the material. They have proposed different angles on which reflectance and transmittance can be observed of nanocone-based solar cell positions. The observation was done on the visible spectrum. The different angles were 0^0, 15^0, 30^0, 45^0 and 60^0 [29].

Chapter 3. Fundamentals of Solar cell

3.1 Basics of the Solar Spectrum

Only the emission of partial part of the net energy of sunlight can be seen as at earth. The formation of sunlight is considered in the form of a visible spectrum of the electromagnetic spectrum. Generally, it is nothing but a form of electromagnetic radiation energy. This can be mentioned as:

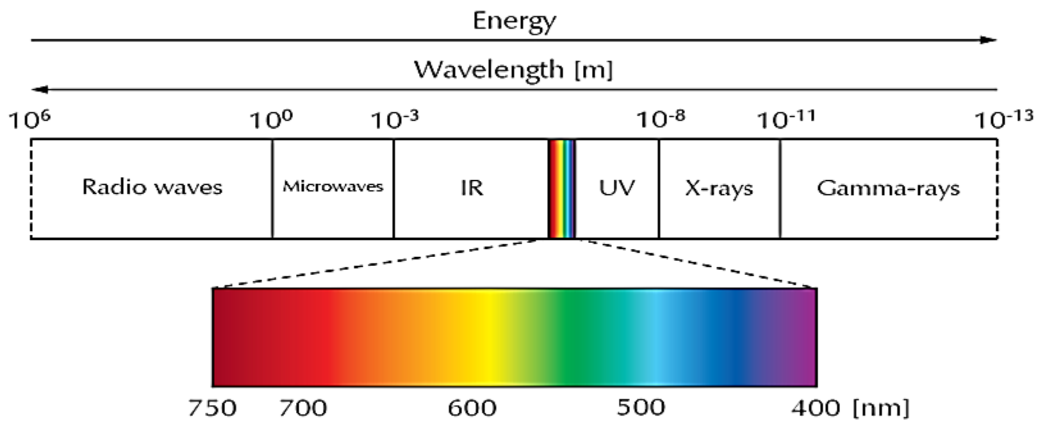


Figure 3.1 The electromagnetic spectrum [6]

The above mentioned EM spectrum has a unique wavelength. According to the Planck proposal, different constituents of energy combined and as a result total energy of light obtained which is known as energy quantum. On the basis of examination of the photoelectric effect that is proposed by Einstein gives different values of subsets of quantum energy and in 1918 and 1921, they won the Noble prize for physics. So, it can be concluded that light can be seen in the form of packets that is known as Photons. In the quantum mechanics, particle nature and wave nature of light are demonstrated. All other particles like protons and electrons, the photon is also characterized in the form of the wave packet. At the spatial position, this wave packet can be treated as a particle. Due to this dual nature of particle and wave of the photon, it is known as “wave-particle duality”. According to this analysis, it can be proved that light is nothing but a form of quantum mechanical particle known as a photon. The information of interaction of sunlight with other object or photovoltaic converter can be determined by different solar energy’s characteristics. These incident solar energy’s characteristics are mentioned below [6]:

1. The incident light's spectrum,
2. The power density of sun radiation,
3. The incident angle between the photovoltaic module and solar radiation
4. The energy which is radiated from a particular surface with some specific time.

3.1.1 Photons

The characterization of a photon can be in the form of energy or wavelength. The relationship between the light's wavelength and photon energy can be shown as [5]:

$$E = \frac{hc}{\lambda} \tag{1}$$

Here, c denotes the speed of light which is 2.998 × 108 m/s and h is the Planck constant equal to 6.626 × 10-34 joules. Then the value of hc = 1.99 × 10-25 joules-m is obtained. According to the above relationship, it can be concluded that red light comes under the long wavelength and blue light is considered in short wavelength. In terms of eV, hc can be written 1.24 eV μm.The energy of a photon can be written as [5]:

$$E = \frac{1.24}{\lambda(\mu m)} \tag{2}$$

3.1.2 Spectral irradiance

The sunlight which is radiated by sun is a part of EM radiation that is Visible, Infrared and Ultraviolet lights. While entering into the atmosphere of earth it gets filtered out and seen as daylight when the sun is up in the skyline. The portion of radiant energy from sun per unit area and time is known as Solar Irradiance. And outside the atmosphere of earth, it depends on wavelength at a point. It is maximum at the range of 0.3 μm to 0.8 μm wavelength. Below is the spectrum of solar irradiance.

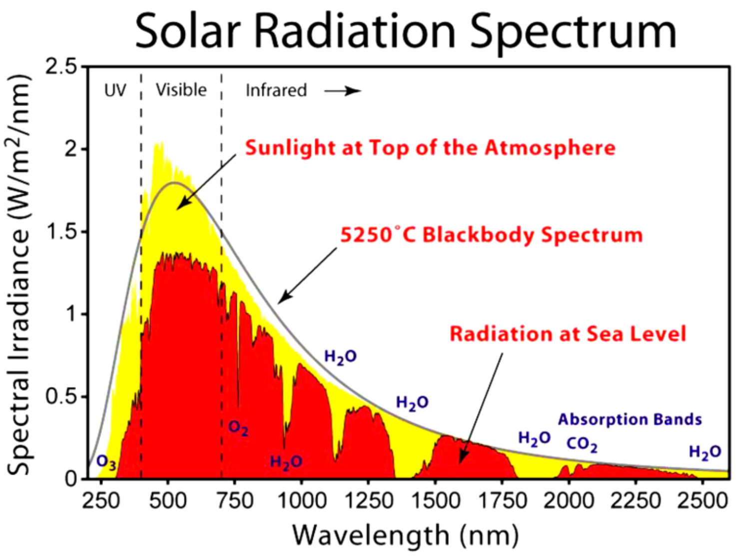


Figure 3.2 Spectrum of Solar irradiance [7].

At about 5,800 degrees Kelvin, this spectrum is similar to that of the black body. The length of the path travel by solar radiations via atmosphere of earth is represented in Air Mass (AM) units which increases with inclination from the horizon [7].

3.1.3 Air mass coefficient

It is defined as the path length of optical rays straight passing through the Earth's atmosphere normalized to the short path length vertically upwards (when sun is at overhead), that is at the zenith. It helps in distinguishing the spectrum of solar rays just after they travelled via the atmosphere. We represents this by the syntax "AM" following by a number. For example, "AM1.5" which define the characteristics of solar rays in the terrestrial region.

It is explained as the immediate length of path covered by optical solar rays via the atmosphere of the earth and is a proportion to the vertically upwards route length which is at the zenith. It describes the nature and properties of the spectrum of solar radiations after traveling through the atmosphere. The syntax is used is “AM” before a number.

Now at angle θ solar radiant light incident in relative to the perpendicular to the surface of the earth and cover the path of length L, then the Air Mass coefficient is [7],

$$AM = \frac{L}{L0} \cong \frac{1}{\cos\theta} \tag{3}$$

Where L0 is the path length from zenith and is normal to the surface of the Earth (at sea level) and θ is in degrees known as zenith angle. AM depends on the elevation path of the sun via the sky. Thus with the passing of seasons and days of the year, it changes accordingly. One more parameter is the observer's latitude which affects it. Beyond the earth's atmosphere which is the outer space, AM0 coefficient is used for defining the solar spectrum. All these are shown below in the figure. At AM0, the solar power comes out to be around 136.6 mW/cm^2. As radiation of the sun travels via the atmosphere, there occur atmospheric attenuation and diffusion.

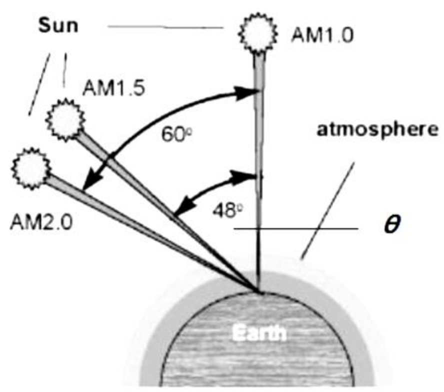


Figure 3.3 Solar Radiation Air Mass standards and corresponding Latitude [7].

At latitude 48.2 degrees Air Mass coefficient with respect to the horizon of the earth is AM1.5G. Here the solar power reduces from 136.6 mW/cm^2 to around 100 mW/cm^2. Most of the solar cell efficiency is observed and measured accordingly. For AM2, the zenith angle is 60 degree as shown above. It is important for the measurement of efficiency or performance of the solar cell in northern Europe which is at higher latitude [7].

3.2 About PN junction

Solar cell can be made up of different materials that are either with a one element, like Si (silicon) or Ge (germanium) or the compounds, like InP, Gallium Arsenide, CdTe (Cadmium Telluride), or the alloy, like $Al_xGa_{(1-x)}As$ and $Si_xGe_{(1-x)}$, where x is from 0 to 1 [5].

3.2.1 Formation of PN junction

- Firstly the material's n type is combined with p type, in that joining process the electrons in excess amount in n type diffuse with the p type and conversely true for the p-type sided material.

- There is holes movement from p-type to n-type which results in the growth of negative ion in it. On the other hand, n-type get the positive ion cores in it, at junction this led to a generation of a potential difference and a depletion region is formed. This potential difference produces an electric field at the junction.

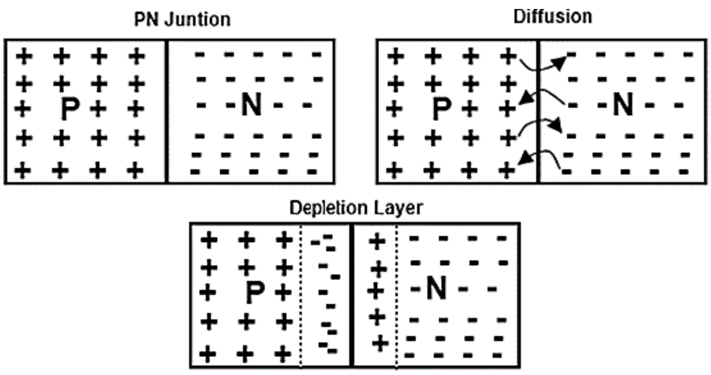


Figure 3.4 Formation of PN junction [8]

3.2.2 Conduction in semiconductor

At low temperatures, they behave as the insulators. Whereas at higher temperatures, they act as conductors. At maximum temperature conduction happens, it is just because of the breaking of the covalent bond among atoms which give them the freedom to move anywhere across the semiconductor. At the higher state of energy only, electrons get an ample amount of energy to take part in conduction. Whereas in a low state of energy, they get bounded and don’t take part in conduction. Hence energy can be introduced between two electrons with the bond that is present among them. Between these two energy levels, no electron can attain the in-between energies. Either electrons can remain at a position having low energy in the bond, or acquire sufficient quantity of energy in breaking the bond or there is a definite amount of minimum energy termed as “Band Gap” of the semiconductor [5].

3.2.3 Band Gap in materials

As we said it earlier that the minimum energy should be acquired by the electron to move away or break free of the bounded state is the Band Gap. There is two levels of energies named as conduction band and valence band. The conduction band is known to have the higher energy level whereas the valence band is the lower level of energy. It can be shown below,

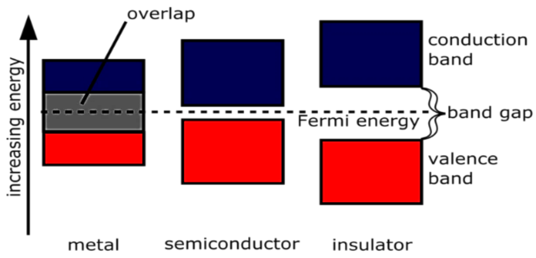


Figure 3.5 Band gap of different materials [9].

When an electron gains energy more than the energy of band gap, then that electron jumps or excite from a low level known as valence band to a higher level band known as the conduction band. Actually, the conduction process in semiconductor relies on the amount of solar energy required by the band gap of the material and the respective amount of energy is generated. Moreover, besides of electrons, holes also take part in conduction. Bandgap exhibit the minimum energy difference among the bands. Whereas, the bottom of the valence band and top of the conduction band are of different value in terms of electron momentum [10], so we have two types of bands based on structure.

1. Direct band gap semiconductor

In this, momentum value of the top of the valence and the bottom of the conduction band happen to be the same value, as shown below.

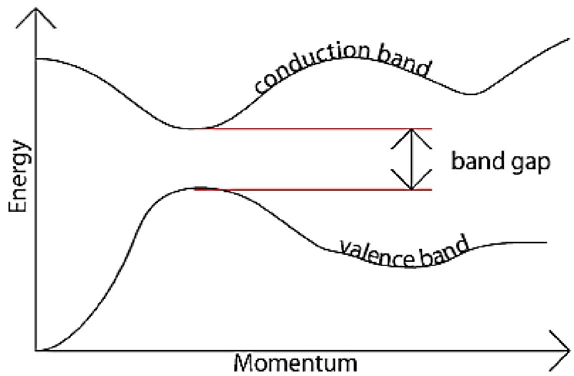


Figure 3.6 Direct bandgap [10].

2. Indirect band gap semiconductor

In this, valence band's higher energy have the different momentum value in respect to the lower energy level in the conduction band.

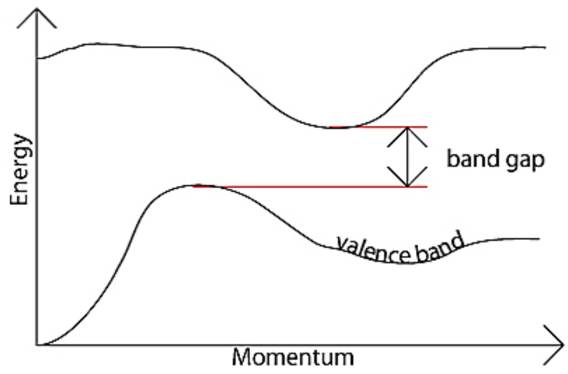


Figure 3.7 Indirect bandgap [10].

A single photon with E energy has momentum p and since the energy of an optical photon lies in the order of 10^{-19}J. Thus a photon has momentum with less amount. The equation is given below [10],

$$p = \frac{E}{c} \tag{4}$$

In a direct bandgap semiconductor material, an electron-hole pair can be generated by photon easily. An electrons do not need much of the momentum. But the same case is not that with the indirect one. An electron must have variations in the momentum for electron-hole pair generation. It can happen only when this electron not only interact to gain energy with the photon but also with the lattice vibration known as Phonon. That‘s why the indirect process is the slower one as it needs three things: a photon, an electron and a phonon to interact.

Hence Gallium Arsenide, CdTe and CdS are used to fabricate LEDs and lasers because they lie in direct bandgap semiconductor whereas Si (silicon) is not, as it is an indirect one.

3.3 Generation of Current Carriers

There are certain following steps that are occurred during current carriers’ generation.

3.3.1 Absorption of light

The conditions for absorption is when the photon’s energy is equal to or more than the band gap of the material, then the absorption of photon by the material occurs and it electrify an electron into the conduction band. Both a majority and minority carriers are

generated just because the absorption of photon takes place. The base for the production of energy required for photovoltaic is the generated charge carriers by photons.
When photons incident on the semiconductor's surface, they can be either reflected, can be absorbed in the semiconductor, or nothing happens and can be transmitted through the material. If photon absorbs, then there may be the possibility of excitation of an electron. Photons falling onto a material can be categorized into three groups which are based on their energy compared with the semiconductor's band gap [5]:-

- If the energy of the photon is less than the band gap of the material, then it passes through the material.
- The hole and electron pair is generated when energy of photon is equal to the band gap of the material.
- The absorption occurs when energy of photon is greater than the band gap of material.

3.3.2 Recombination

The electrons possesses meta-stable state when they are present in the conduction band. Electrons becomes stable when they move to their valence states. Also, hole generation takes place upon stabilization of electron. This phenomenon is referred as recombination. Basically, there are following three types of recombination [5]:

(a) Radiative Recombination

Light produced in LED is an example of radiative recombination. Space solar cells and Concentrator are made with the help of materials having direct bandgap and radiative recombination dominates there. However, there are multiple terrestrial solar cells which are composed of silicon, these are indirect bandgap semiconductors. There are few following characteristics of radiative recombination [5]:

- Direct combination takes place between hole from valence band and electron from conduction band.
- After this recombination of electron and hole, photon emission takes place. The energy of the photon is similar to the energy gap of the material and hence, photon gets weakly absorbed so that it is capable of exiting from semiconductor.

(b) Shockley Read Hall Recombination

This is basically a recombination that takes place through defects. It occurs in those materials which are not pure. There are following two steps involved in this recombination [5]:

- Inside material defects, energy can be trapped by a hole or an electron. The defects are introduced in the material by addition of different element, such as material doping.
- Recombination of a hole and an electron takes place if hole and electron are into the same energy state before the thermal re-emission of electron into conduction band.

(c) Auger Recombination

There are three carriers involved in this type of recombination. After recombination of a hole and an electron, if energy is neither emitted as heat not photon, instead if the energy is fed to the electron, third carrier in the conduction band. It is caused when the concentration of carrier is high due to injection at high level during concentrated sunlight or due to heavy doping. The lifetime is limited in Auger recombination in Si solar cell. Auger recombination lifetime is inversely proportional to the doping concentration in the material [5].

3.3.3 Movement of carriers

- These carriers move freely in the semiconductor lattice in a random direction with some velocity.
- There is no net overall movement of carriers in any direction.
- Electrons in the conduction band and holes in the valence band are considered as "free" carriers as they can make crystal lattice [5].

3.4 Working principle

To extract power, voltage as well as current need to produce. Its working principle is a “photoelectric effect”. At junction of semiconductor, there is a collection of light generated carriers which results in the movement of holes to the p-type and electrons to n-type. As carriers come out of the device as a current, so no charge build-up is there.

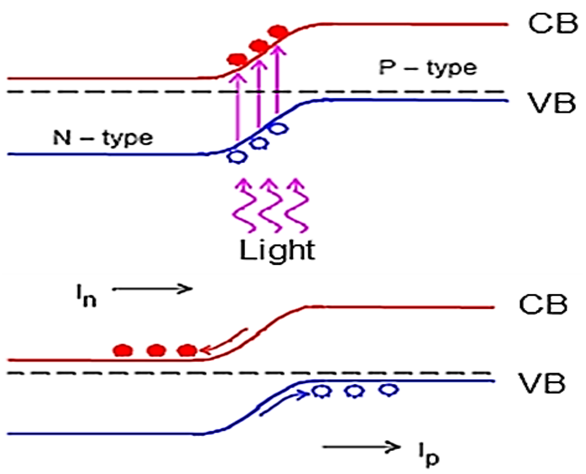


Figure 3.8 Process of power generation [5].

However if these carriers force to remain in the cell, then it can lead to increase in a number of electrons on the n-type side and same as on p-type side with holes. This will generate an electric field due to the separation of charges which will be opposite to the existing field, hence net electric field reduces. An equilibrium exists results in generation of a voltage across the junction of p-n semiconductor [5].

3.5 Equivalent circuit and equations

If solar cell is represented in terms of equivalent circuit diagram. It will look like below figure:

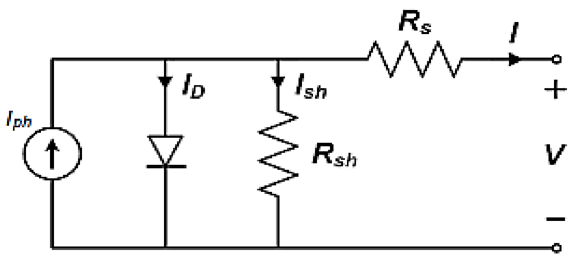


Figure 3.9 Equivalent circuit diagram [11].

Where, I_{ph} = Photon current source, I_d = Diode current, R_s = Resistance encountered by the flow of charges (electrons and holes), as it moves to the bulk material. R_{sh} = Shunt resistance, it represents recombination of electron-hole pair. (Ideally, it will be large). By applying network theorems, we get the following equation [11],

$$I_{ph} - I_o\left(e^{A(V_L+I_L R_S)} - 1\right) - \frac{V_L+I_L R_S}{R_{sh}} = I_L \tag{5}$$

Where, $A = q/\gamma' kT$ and γ' = constant different for different material, k = Boltzmann constant, T = temperature. Above equation relates voltage and current equation.

3.6 Parameters of Photovoltaic Cell

3.6.1 I-V characteristics

These characteristics are the superposition of the I-V curve with the light-generated current of the solar cell diode in dark. There is an effect of light that shifts the IV curve to the 4th quadrant, from where we can get the power from the diode. Solving the above equation (5) using the Newton-Raphson method. Following graph is obtained [5].

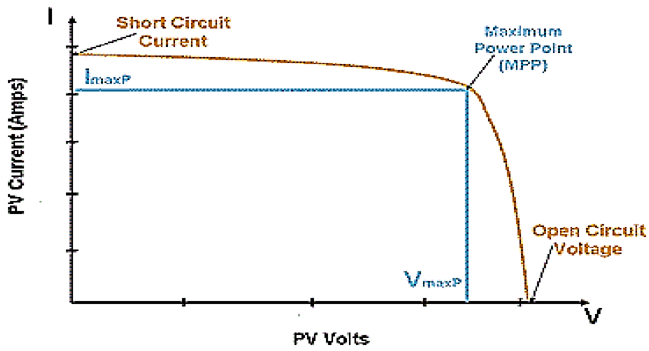


Figure 3.10 I-V characteristics [5].

3.6.2 Short-circuit current

In the solar cell, when voltage becomes zero then the current is termed to be short-circuit current. And represented by Isc. It is the situation when the solar cell is a short-circuited. It is shown below.

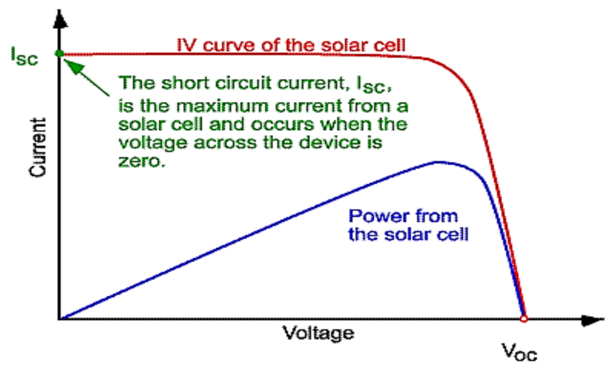


Figure 3.11 I-V curve of a solar cell showing the short-circuit current [5].

Generation and followed by collection of light generated carriers makes this short-circuit current. In an ideal case, the short-circuit current and the light-generated current both are same. Thus, we can say that it is the largest current that can be extracted from the PV cell.

3.6.3 Open-circuit voltage

In the solar cell when current becomes zero then the voltage is termed to be the maximum voltage. Because of the biasing of the junction of the solar cell with the light-generated current shows the amount of forward bias in the form of open-circuit voltage. It is shown on the I-V curve below.

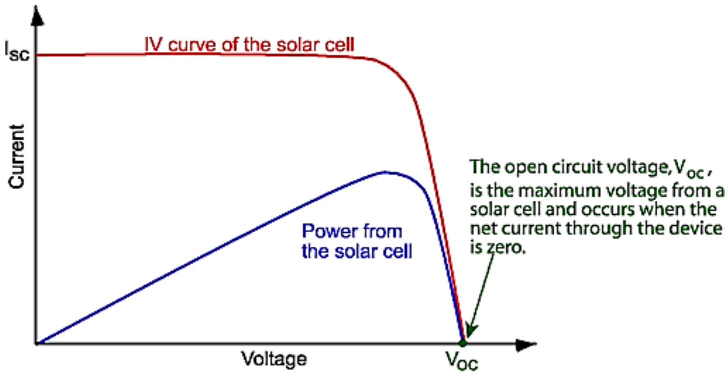


Figure 3.12 I-V curve of a solar cell having the open-circuit voltage [5].

3.6.4 Fill Factor of solar cell

The open-circuit voltage and short-circuit current are the maximum voltage and current from a solar cell respectively. At these operating points the power value is zero. This fill factor can be abbreviated as "FF", and defined as the parameter, which estimates the maximum power extracted from a PV cell. It is the ratio of the maximum power from the solar cell to the multiplication of V_{oc} and I_{sc}. When seen in the graph, it can be shown as the estimation of "squareness" of the PV cell and also defined by the area of the biggest rectangle which can be fit in the curve. It is explained below graphically.

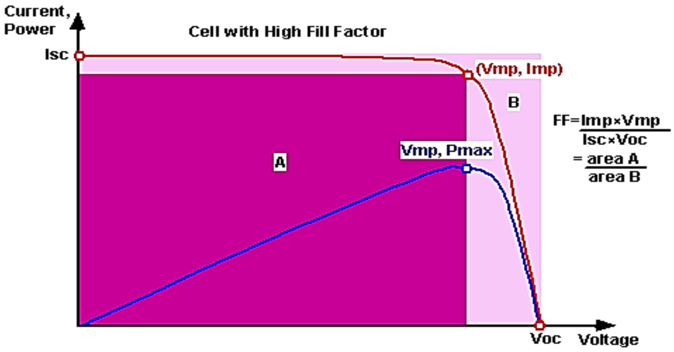


Figure 3.13 Fill factor in graph [5].

In the graph, the red line shows a point having the coordinate (Vmp, Imp), when this point makes a perpendicular contact with axes then an area comes out which is the dark pink area that is ‘A’. And the area ‘B’ is related to the Voc and Isc values as shown above.

3.6.5 Efficiency of PV cell

A parameter is needed to make a comparison between the performances of a solar cell with the other one. It is the proportion of output energy given by solar cell with the energy incident from the sun. Its efficiency relies on the amount and the spectrum of the incident light and also on the solar cell’s temperature. Thus, there must be controlled conditions. Under AM1.5 conditions, Terrestrial solar cells can be measured and at 25 degree Celsius of temperature. For space, AM0 conditions are used. It is defined as [5]:

$$P_{max} = V_{oc} I_{SC} FF \quad (6)$$

$$\eta = \frac{V_{oc} I_{SC} FF}{P_{in}} \quad (7)$$

Where, V_{oc} is open-circuit voltage,

I_{SC} is short circuit current,

FF is the fill factor, and

η is efficiency.

The input power we use for calculation of efficiency is around 100 mW/cm^{2}or 1 kW/m^2.

Chapter 4. Thin Film Based Solar Cells

4.1 Introduction

Three distinct generations of solar cells can be categorized. The 1st generation solar cells are also known as standard or traditional cells, are made up of 200 μm to 300 μm silicon. The two primary constraints of conventional solar cells are: efficiencies and their high production costs. Approximately 70% of the incident radiation energy is lost in the cell. The largest effectiveness reported for mono-Si solar cells in the PV industry is 25%. 2nd generation PV cells are thin film solar cells which consists of amorphous cells of Silicon, Cadmium Telluride (CdTe) and Copper Indium Gallium Selenide (CIGS) that ranges from 1 μm to 2 μm in thickness and get placed on substrates like glass, stainless steel or plastic. Thin film solar cells decreased the price of photovoltaic systems in bulk materials, but radiation absorption in such solar cells is quite low [12]. However, more effective light trapping methods are needed for better efficiency in comparison to wafer-based solar cells in thin films. Regular methods like surface texture used for light trapping in wafer-based solar cells cannot be applied to thin film PV cells; texturing at micron level is comparatively big, while the texturing at the submicron level also invariably improves the surface area and therefore the recombination of the minor carrier on the surface [13].

Therefore, to enhance the absorbance, it is necessary to confine the peak light into the semiconductor. Solar techniques of the third generation use sophisticated thin film cells. Compared to other techniques, they generate comparatively high effectiveness even at a low price. Localized surface plasmon resonance (LSPR) due to metal NPs is a promising way to increase light absorption in thin-film PV cells that forms the plasmonic solar cells (PSCs) [12].

Materials that can be used worldwide for fabricating thin films are Cadmium Telluride, Copper Indium Gallium, Silicon and Gallium Arsenide. First three are used for commercial purpose while the Gallium Arsenide is used for spacecraft purpose. As they are the most expensive one but has the highest efficiency of around 28.8 %. They are commonly used for multi-junction solar cells [14].

4.2 Fundamentals of Absorption, Transmission and Reflection

Three procedures happen when radiant flux incident on a surface or medium: transmission, absorption, and reflection. Below figure represent the ideal case. Along with them, scattering and emission also occur but in very less amount, so we deal only with the above three. The components of Transmittance and reflectance are either specular or perfectly diffuse which is shown below [15].

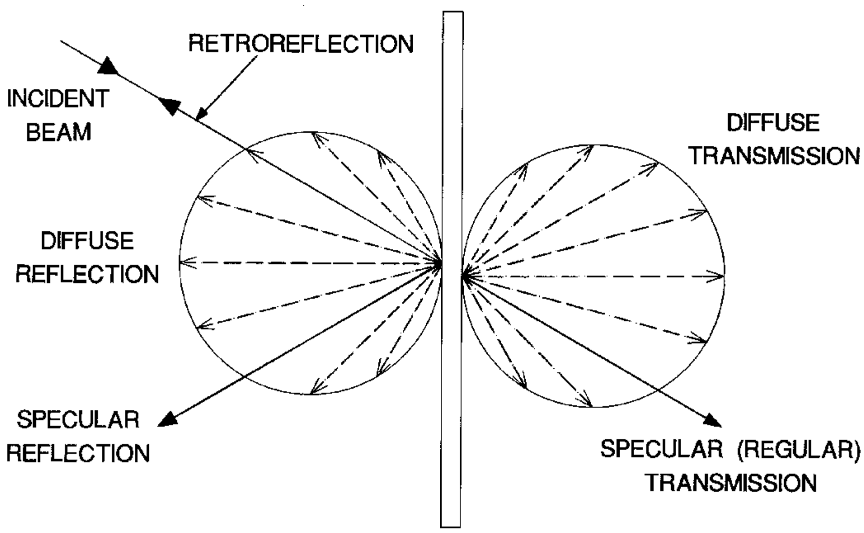


Figure 4.1 Idealized reflection and transmission [15].

Now let's define the specular and diffuse terms in regarding of reflection. Specular reflection is produced by a smooth surface. The angle of incidence and angle of reflection are equal. Thus specular materials produce images on their surface as a mirror does. Whereas diffuse reflection is produced by rough surfaces. In this, the incident angle created by the light ray makes a multiplicity of reflection angles [16]. Now there is a difference between the suffixes we use that is –ance and –ivity. The terms ending with –ivity such as absorptivity, reflectivity, transmissivity are describing the property for pure materials. Whereas the suffix –ance is used for characterization of a specimen or sample [15].

4.2.1 Transmittance

It is the term defining the process in which the incident light or radiant flux travels through a surface or medium from the non-incident side, usually the other side. The spectral transmittance $\tau(\lambda)$ of a medium is the proportion of the transmitted spectral flux ϕi to the incident spectral flux ϕt [15],

$$\tau(\lambda) = \frac{\phi i}{\phi t} \tag{8}$$

Now the transmittance τ can be defined as the ratio of transmitted flux ϕI to that of the incident flux ϕt or [15],

$$\tau = \frac{\int_0^\infty \tau(\lambda)\phi i \, d\lambda}{\int_0^\infty \phi i \, d\lambda} \neq \int_0 \tau(\lambda) \, d\lambda \tag{9}$$

4.2.2 Absorptance

It is the process in which the incident radiant light or flux is converted to another form of energy or heat. It is the fraction of the incident light or flux that is absorbed. It is denoted by α and is defined by α = ϕa/ϕi. Just as same, the spectral absorptance α (λ) is the ratio of spectral power absorbed ϕa to the incident spectral power ϕI [15],

$$\alpha = \frac{\int_0^\infty \alpha(\lambda)\phi i \, d\lambda}{\int_0^\infty \phi i \, d\lambda} \neq \int_0 \alpha(\lambda) \, d\lambda \tag{10}$$

An absorption coefficient α' (cm-1 or km-1) is used in the equation τi = e- α't, where τi is the internal transmittance and t is the length of the path (cm or km).

4.2.3 Reflectance

It is the process in which a fraction of the radiant flux or light incident on a surface is throwing back to the same hemisphere whose base is the surface having the incident radiation. The reflection can be specular or diffuse or both.

Generally, the definition for reflectance r is the ratio of the radiant flux reflected ϕr to that of incident radiant flux ϕi [15]

$$r = \frac{\phi r}{\phi i} \tag{11}$$

Whereas spectral reflectance is similarly defined at a specified wavelength λ as [15],

$$r(\lambda) = \frac{\phi(\lambda) r}{\phi(\lambda) i} \tag{12}$$

4.2.4 Relation between Transmittance, Reflectance, and Absorptance

Radiant flux or light fall upon a medium or surface undergoes a reflection, transmission, and absorption. Conservation of energy has an application that leads to the statement that the sum of the reflection, transmission, and absorption of the incident light is equal to unity, or [15],

$$\alpha + \tau + r = 1 \tag{13}$$

In the absence of nonlinear effects (that is Raman Effect, etc.) [15],

$$\alpha(\lambda) + \tau(\lambda) + r(\lambda) = 1 \tag{14}$$

From the above equations, we conclude that if one or two quantity is minimized then the other quantity can be increased. For example, by minimizing the reflectance and transmittance, we can actually maximize the absorption [15].

4.2.5 Absorption coefficient

The photons in the incident light having higher energy than the band gap energy of the absorber material get transmitted away from it. This is due to the thickness of the absorber medium which is an insufficient one. Now at a given wavelength, the length requires to absorb the photon is called an absorption length. To absorb all radiation, the thickness of the material should be equal to the absorption length of the photon of energy which is equal to band gap energy. Thus the thickness of material d is given by [17],

$$d = \frac{1}{\alpha(Eg)} \tag{15}$$

Where, $\alpha(Eg)$ is the absorption coefficient of the photon with energy Eg of the band gap.

4.3. Light trapping

2nd generation thin films solar cell is better than the first generation's crystalline silicon-based solar cell in terms of factors like low material consumption, lesser energy payback period, monolithic integration, large area modules, tuneable material properties, low-temperature processes, transparent modules can be made. With these advantages, they lack at one point that is their low solar efficiencies due to poor absorption properties. One of the factors is the width of the active layer which lies in the range of few nanometers (nm) to several 10s of micrometers (µm). If there is a requirement of minimizing the thickness of material which is an absorber, then it is important to increase the length of the path of solar rays of the solar radiation in that absorber material in respect to decrease the transmission losses. The length which an unabsorbed solar radiation will have to travel in a cell before it gets out from it is known as the optical path length. And this can be enhance by a technique known as light trapping. For efficient absorption, light needs to be trapped more and more [17].

In the thick substrate solar cell, rays of light are traveling normal to the surface will have an optical path length equal to the device's thickness. For an increment of the optical path length, it needs to change the angle of incidence for the light. That led to an increase in optical path length. Moreover, the rear surface should be a reflector of having a well-textured surface. So that TIR occurs and rays reflect within the volume of device as shown in the figure. TIR (total internal reflection) can occur when light travels from high refractive index n_2 to low refractive index n_1. Explained by Snell's law [17]:

$$n_1 \sin\theta_1 = n_2 \sin\theta_2 \quad (16)$$

For TIR, θ_2 in the above equation should equal to zero, and θ_1 should be a critical angle [17].

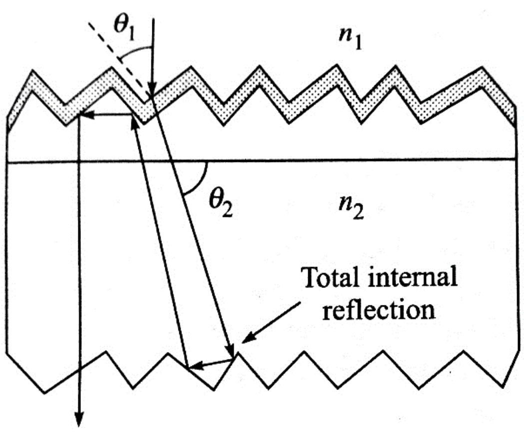


Figure 4.2 Scheme of light trapping in a solar cell [17]

Above is the basic concept of trapping the light, but it is true only for thick solar cell. Also, there is a thermodynamic limit being set for thick films by the absorption increasing factor of $4n^2$, and n is the refractive index of the film. It is known as the Lambertian limit. And if operated at nanoscale structure then it can exceed or eliminate.

[26] For thin film solar cells, these schemes have to be changed or modified due to practical difficulties in implementing large textured structures at the rear, and different basic optical characteristics of thin films [18]. So, there are various techniques of trapping the optical light in the thin film solar cell. Which are as follow:

1. By using gratings,
2. By using nanostructures, and
3. By reducing the surface plasmonic absorption.

Use of diffraction gratings in a solar cell affect its efficiency. For example, they can be used as a backside grating to scatter the incident solar light to wider propagation angles afar from the angles of TIR. This can make an increment in the interaction length of photons with long wavelength inside the active layer and thus increase the efficiency [20].

4.3.1. Light trapping using Plasmonic absorption

Plasmonics is a significant component of nanophotonics ' intriguing field, exploring how electromagnetic (EM) fields can be restricted over dimensions at or below the wavelength. Its principle is the interaction between the radiations of the electromagnetic wave and the conduction electrons at interfaces of metallic or in a metallic structure at the nanoscale, resulting to an increasing optical near field of subwavelength dimension [21].

If this metallodielectric structure is engineered properly, then light can be collected and trapped in the thin film layer. And increase absorption accordingly. There are two phenomena responsible for it. One is localized surface plasmons electrified in metal nanoparticles. And the other one is the surface plasmons polaritons (SPPs).

Plasmonics in PV

In thick films, maximum region of the solar spectrum which is of the range of 600-1100 nm, is absorbed poorly by it. These traditional solar cells have a much larger thickness of range 180-300 µm. but for good absorption, they should have diffusion length of minority carriers to be in multiple times the thickness of the material, so that all the photocarriers can be collected. Whereas in thin films, this condition eliminated or won't happen [22].

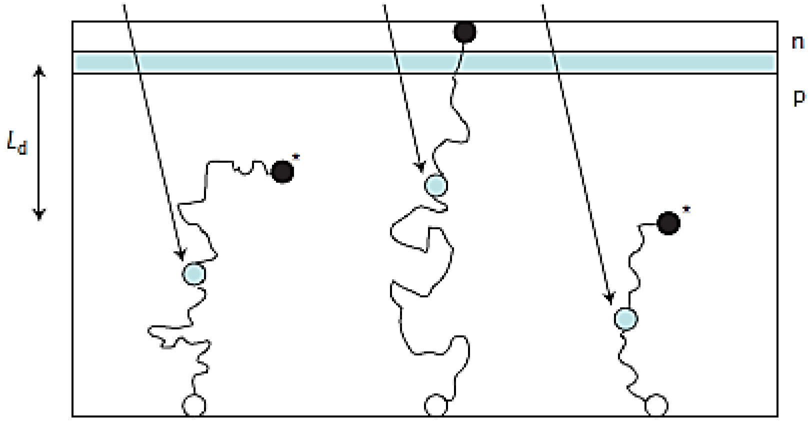


Figure 4.3 Diagram shows the carrier diffusion from the photo-generated region [22].

In the above figure, generation of charge carriers occurred at the region which is at longer distance away from the p-n junction. And they are not collected or assembled at one place effectively regardless of the bulk recombination. The region of the generation which is far away is more than the diffusion length L_d. The structure with plasmonic effects can give us the option of decreasing the thickness of the absorber layer while making the optical thickness constant in three ways. They are:

1. Using subwavelength scattering elements like metal nanoparticles to bind and couple the EM waves from the sun which propagate freely into the absorber layer of thin film.It is shown below.

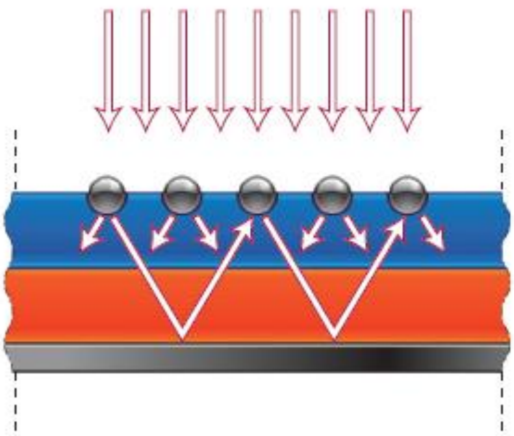


Figure 4.4 Light incident on the device and get trap by scattering from the metal NP at the surface only. It is scattered and trapped in a thin film by high scattering angle and at multiple times results in increment in optical path length [22]

2. Using a subwavelength antenna like metallic NPs, effective absorption can be increased via coupling of the plasmonic near field with the semiconductor. It is shown below.

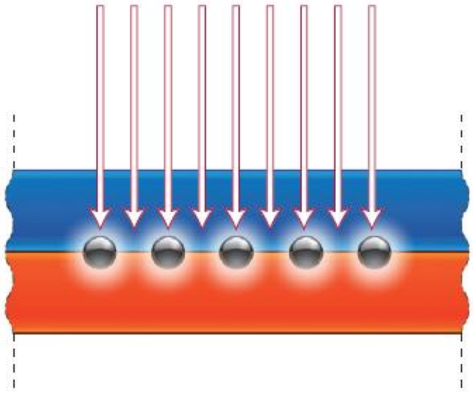


Figure 4.5 Localized surface plasmons get excited in metal NPs embedded in substrate to trap the light. Those excited particles' near field results into generation of electron-hole pairs in an active layer [22].

3. Using a channeled film of metallic on the rear surface of an absorber layer can trap light into SPP mode bearing at the interface of metal and semiconductor and also guided modes in substrate slab, where the light is transformed into photocarriers in substrate.it is shown below.

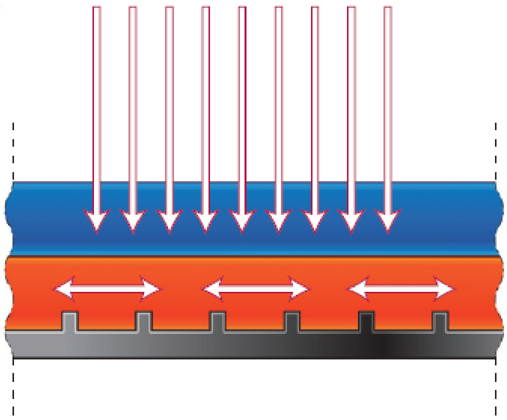


Figure 4.6 Surface plasmon polaritons are excited at metal at the interface of metal and semiconductor trap the light. This metal surface couples photonic mode or SPP to light that travels in the plane of an active layer [22].

Localized Surface Plasmon Resonance (LSPR)

It is the event in which conduction electrons oscillate collectively nearer to the metal surface under the effect of an external electromagnetic field and it can excite via metallic NPs like aluminum, silver, copper, and gold. The SPR wavelength relies on the size, material, and geometry of the NP array. It also depends on the refractive index of that media. To fully make use of the sun's light for high efficiency of the solar cell, the scattering of light is more important than the absorption of light by metal NPs [22].

Scattering and absorption by metal nanoparticles

Due to the presence of metal NPs, plasmonic solar cell functions well which includes absorption and scattering of light. Metal nanoparticles scatter the incident light from the sun across the surface of the active layer at resonance wavelength. The cross sections of scattering and absorption is given by [12]:

$$C_{scat} = \frac{1}{6\pi}\left(\frac{2\pi}{\lambda}\right)^4 |\alpha|^2; C_{abs} = \frac{2\pi}{\lambda} Im|\alpha| \tag{17}$$

$$a = 3V \frac{\omega_p^2}{\omega_p^2 - 3\omega^2 - I\omega\gamma} = 3V \left[\frac{\frac{\varepsilon_p}{\varepsilon_m} - 1}{\frac{\varepsilon_p}{\varepsilon_m} + 2}\right] \tag{18}$$

Where α is the polarizability of the metal particle with V volume, ε_p is its dielectric function and ε_m is a dielectric function of that medium in which NP is embedded. If $\varepsilon_p = -2\varepsilon_m$ then its polarizability will be large. It occurs when frequency nearly equal to SPR ω_{sp}, which allow the light to interact with the area larger than cross-section of particle. Surface plasmon for spherical structure occurs at $\omega_{sp} = \sqrt{3}\omega_{sp}$ [12].

When light scatters from a metal NP embedded in homogenous medium, it travels nearly symmetric in forward and reverses directions. Now situation changes if it placed close to the two dielectric's interface. Their light will prefer to travel into the dielectric which would have higher permittivity. That scattered light gains an angular spread in dielectric which led to an increase in optical path length. Due to angle beyond the critical angle for reflection and presence of metal reflector on the backside, the light will remain in the active layer. Hence the effective path length of light increase [22].

Regarding the materials' plasmonic effects, gold is stable and shows resonant frequency in the visible region with a broader peak. Silver and aluminum is also good enough for this but gets oxidized, that changes the resonance frequency. But they are cheaper than gold. Thus, different materials with different dimensions can be used to increase the thin film solar cell's efficiency [12].

Chapter 5. Simulation Design and its Results

5.1 About Structure

We have proposed the structure having three thin layer films placed one on another. And metallic nanoparticles are embedded in them. For solar applications, we have coupled these thin films with the nanoparticles. And try to optimize the proposed structure by changing the dimensions of the structure. But before designing, there should be a basic understanding of the materials and software we are going to use.

5.1.1 Materials used in the structure

1. Gallium Arsenide (GaAs) - It belongs to the III-V group in the periodic table. There are many other compounds like InP, AlAs and GaP that also belongs to this group. Their atomic structure is the same as that of the Si atomic structure. The number of atoms of Ga and As are the same in their lattice structure. Various properties of III-V compounds are better than silicon one. Thus they are the best option for electronic materials. But they are too costly. The properties are:

- These compounds are direct band gap semiconductors. They have a high absorption coefficient. Thus beneficial to use them for thin film layers for solar spectrum absorption. Its absorption coefficient is about$10^5 cm^{-1}$ at 550 nm wavelength.
- Its band gap is nearer to the ideal band gap. That is 1.42 eV.
- It is possible to vary the composition of the crystal. This results in a change in the band gap with replacing some atoms with the other atoms of the group 3rd or 5th.
- Refractive index at 632.8 nm wavelength is 3.85 [17].

2. Indium tin oxide (ITO) - It is used here as a transparent conductive oxide (TCO). In case of a thick Si wafer-based solar cells, charge carrier travels a long way in the emitter to reaching to contacts. It became possible only because of the conductivity of Si wafers used have a high value. But this is not the case of thin film materials. Its dark conductivity is worst and due to this transportation of charge carriers won't happen. For efficient charge collection, a metal contact with continuity on the front surface is needed. But it should be transparent so that a large amount of light can enter the cell. Hence the function of continuous and transparent metal contact is completed by TCO.

Properties of good TCO are:

- Conductivity should be as high as possible. It affects the cost and design of thin film PV cells.
- Transparency of the material should be as high as possible. So that no optical loss would be there. The layer should provide the lowest reflection when used as a front layer. And it should be according to the below equation [17]:

$$d_{tco} * n_{tco} = \frac{\lambda}{4} \quad (19)$$

Where n_{tco} is the refractive index of TCO layer and λ is wavelength at which reflection needed is minimum.

ITO completes the TCO layer's requirements. And the best option to be used it as a front layer. Its band gap is 3.7 eV. And its refractive index is around 2. And it has around 95 % of transmission compared to the other TCO materials [17].

3. Nanoparticles – particles at nanoscale. They have dimensions less than 100nm. NP compose of 3 layers that are a surface layer, shell layer, and the core. These are distinguish into various categories. Which are carbon-based NPs, Metals NPs, ceramics NPs, Semiconductor NPs, and polymeric NPs. our main concern is of metal NPs only, which shows optoelectrical properties due to the presence of LSPR. It have only alkali and noble metals that are Cu, Au, and Ag. They have a wide absorption band in the visible region of the spectrum. They are widely used nowadays due to their advance properties [23].

5.1.2 Simulation software used

The OptiFDTD simulation tool is a highly integrated software which is used for computer-aided design and moreover, passive photonic components can be simulated. This software is based on the method known as the FDTD method. An engineering tool for powerful simulations of diffractive optics device. It has unique features, like the potential to model propagation of light, diffraction, and scattering, polarization and reflection effects.

FDTD (Finite-difference time-domain) method – It is the best method to solve numerically the differential equations. The two Maxwell's curl equations that are Faraday's and Ampere's laws can be discretized by using the central difference approximation. And then solve the outcome equations to get the electric and magnetic field distributions.

5.2 Simulation Results and Analysis

In this thesis for improvement of coupling in thin films via using metal nanoparticles, the structure that is proposed is having a thick 250 nm Gallium Arsenide (GaAs) layer, an ITO (Indium Tin Oxide) layer of 70 nm, and Al (Aluminum) layer of 70 nm. Metal nanoparticles are planted into the ITO coating with the period of p=150 nm and also in contact with the GaAs layer [24]. Which is shown below,

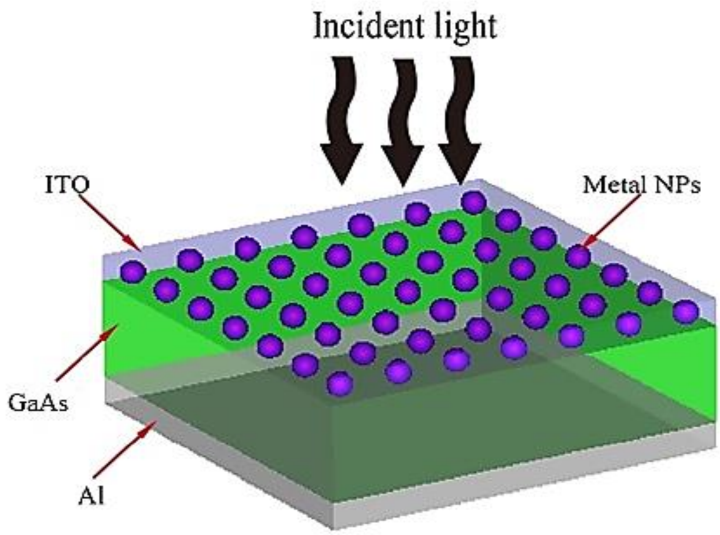


Figure 5.1 3-D model of the solar cell having thin films and metal nanoparticles [24].

Our aim is to enhance the optical absorption in the proposed structure. It would be beneficial for the solar cell applications an increase in the optical absorption will enhance the efficiency of the PV cell. So we would focus more on the absorption characteristics of thin layers for different microstructures of the model having metal nanoparticles in it. and that can be achieved by varying the affecting parameters that include the shape, material, and size of the nanoparticles. For this work, OptiFDTD 32-bit by Optiwave software is used for simulation. Above structure is designed in its layout which is shown below:-

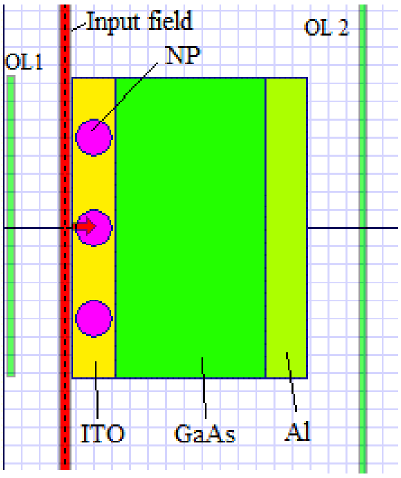


Figure 5.2 Layout diagram of thin film solar cell structure in Optifdtd designer.

In the above figure, NP is the nanoparticles and here three nanoparticles are embedded in ito with the defined period p=150nm. They are modeled using the Drude-Lorentz model. The incident rays from the sun would be in the form of field and here the red line is used for this purpose. This red line is actually Input field wave source. For this simulation, a Gaussian modulated EM(electromagnetic) plane wave source which is linearly polarized is used. The center wavelength is at 600 nm. The input power used has an amplitude of 1 V/m. The direction of input fields is in the Z direction as our layout designed in the X-Z plane. Now we have placed two observation vertical lines that are OL 1 and OL 2. Observation vertical line 1 is used for extraction of reflectance whereas Observation line 2 for transmittance power spectrum.

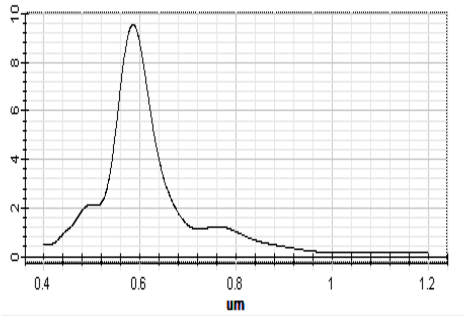
Now we have analyzed the reflectance and transmittance power at the centered wavelength and also on different wavelength ranges. As this is helpful estimating roughly about the absorption in the solar cell. According to the 13^{th} equation, If both reflectance and transmittance come out to be minimum then we can say that more absorption is occurring in the solar cell and more absorption of light in the active layer of the solar cell, more the GaAs solar cell is efficient one.

So our motive is to coupling the thin film active layer with the nanoparticles to get the optimal solar cell structure. We have done the material, size optimization and then the various arrangement is applied to optimize the structure. Our aim is to get the minimum reflectance and transmittance power spectrum for the optimized structure.

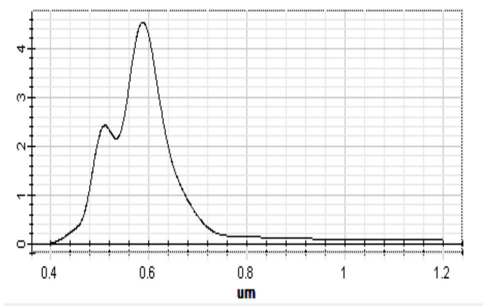
5.3 Reflectance from the structure

5.3.1 Material Optimization

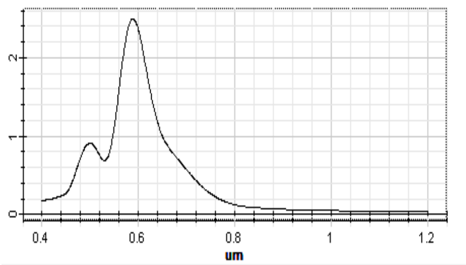
Below are the observed graphs on the optical line 1 where there should be minimum reflections from the front of the structure. These graphs are between the power spectrums of reflectance versus wavelength for different materials like Al, Ag, Au, Cu and also with no NP.



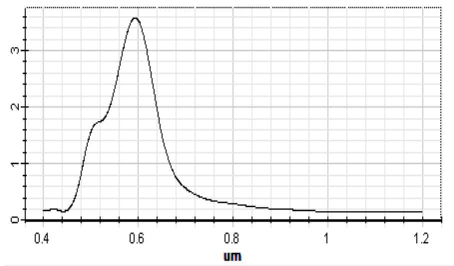
No NP



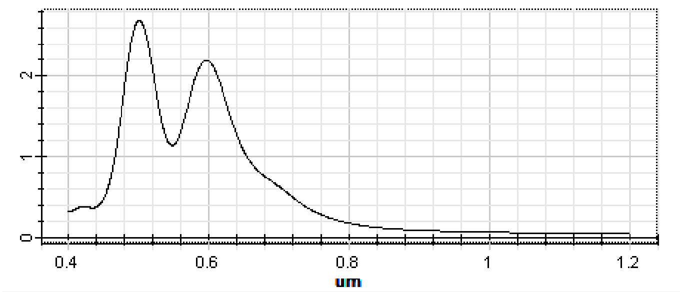
Cu NP



Au NP



Al NP



Ag NP

Figure 5.3 Reflectance versus wavelength graph for the structure with different embedded nanoparticles.

At centered wavelength 600 nm, they show different values as shown in the table.

Table 1.Power spectrum of Reflectance of different metal nanoparticles.

Metal Nanoparticle	The power spectrum of Reflectance (W/m)
No NP	8.75
Al	3.53
Ag	2.18
Cu	4.24
Au	2.35

Now, if we combine all the graphs for comparison .then it will be like the below figure. In this, we observed that when no NP is embedded in the structure, it shows the maximum peak of reflectance between the wavelength ranges of 550 nm to 650 nm. Then followed by Cu NP and Al NP. Then minimum reflectance is shown by Gold (Au) and silver nanoparticle. Where Ag NPs shows the minimum in the 550 nm to 600 nm range and after that they overlap with each other. Hence, Ag NP embedded in the ITO layer show minimum reflection in the visible region of the EM spectrum. It can conclude that the better choice to maximize the coupling efficiency of the active layer is via using silver NP.

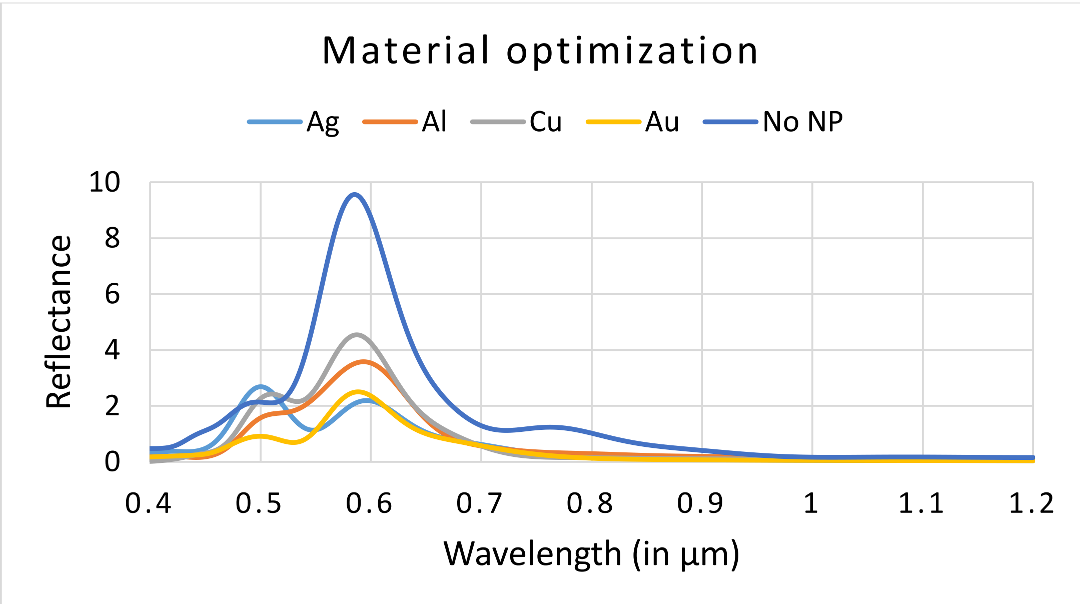
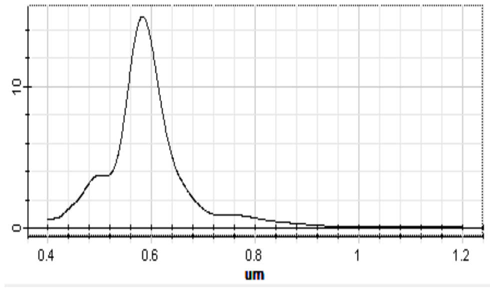


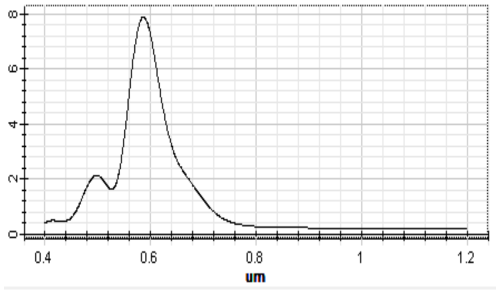
Figure 5.4 Comparison of the power spectrum of reflectance for different nanoparticles.

5.3.2. Size Optimization

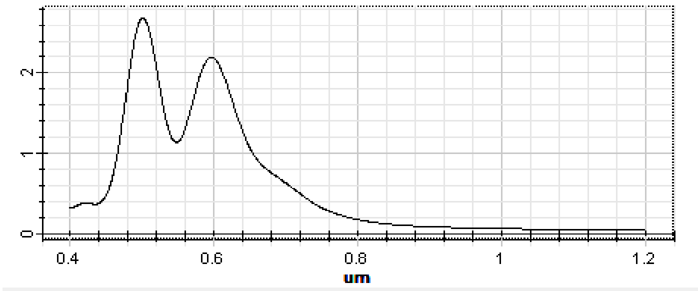
Here we analyze the reflectance characteristics for different sizes of optimized nanoparticle i.e. Ag (silver). We observe different graphs of reflectance for different sizes that are 10nm, 20nm, and 30nm. Below are the graphs,



10 nm



20 nm



30 nm

Figure 5.5 Reflectance versus wavelength graph for the structure with different sizes of Ag NPs.

At centered wavelength 600 nm, they show different values as shown in the table.

Table 2. The power spectrum of Reflectance for different sizes of Ag nanoparticle.

Nanoparticle radius (in nm)	The power spectrum of Reflectance (W/m)
10	12
20	7.19
30	2.18

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It can be concluded from the table that with an increase in the size, reflectance decreases and we can't increase the radius above 30 nm as the ITO layer is 70 nm thick. Below is the comparison graph of a different plot of different sizes of NP.

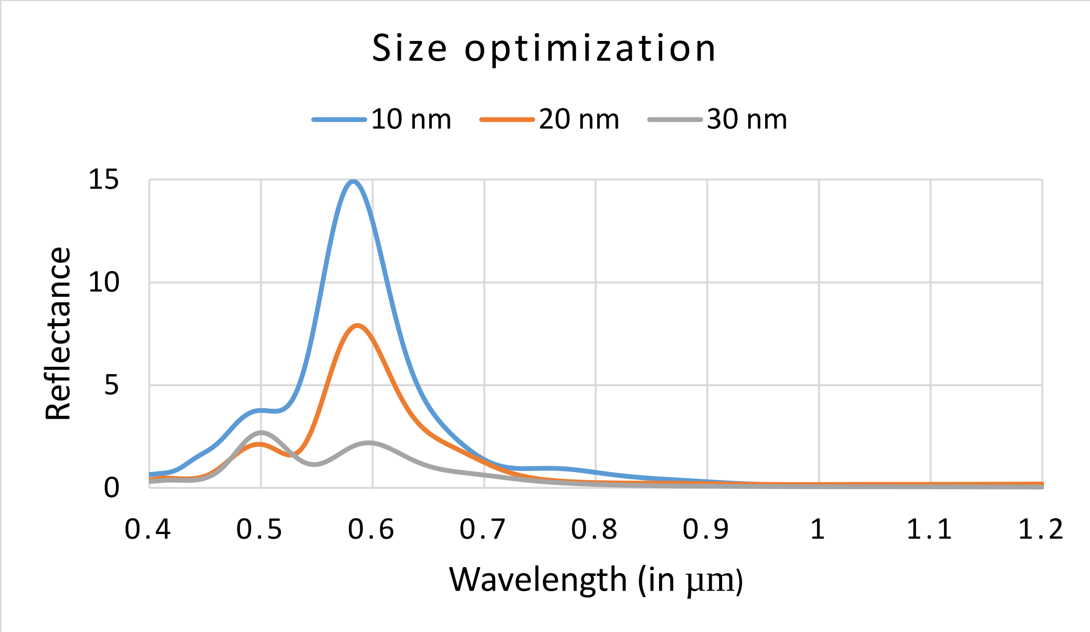


Figure 5.6 Comparison of the power spectrum of reflectance for different sizes of Ag NPs.

Here it can be observed that between the wavelength ranges of 550 nm to 700 nm, Ag NP with the 30 nm radius has a very low level compared with others. Also, it can be said that minimum reflectance is observed in the visible region. That means more absorption of solar radiance can occur because of the low reflectivity. So the structure is optimized with the Ag NPs with 30 nm radius.

5.3.3 Arrangement Optimization

After material and size optimization, the position of Ag NPs are arranged at four different locations as shown in the figure. First, all three NPs at a definite period are arranged in the ITO layer. The structure which is used for the above two optimizations. Then, they have been positioned at the top of the Gallium Arsenide (GaAs) layer with equal spacing and radius nearer to the ITO layer. After finding the results, we again change the position of NPs, by placing them at the bottom of the GaAs layer. And at last, by observing these different positioned structures, we have placed them in the ITO layer and as well as at the bottom of the GaAs layer. But now their radius is different, in the GaAs layer we have not the limitations of as such had in the ITO layer.

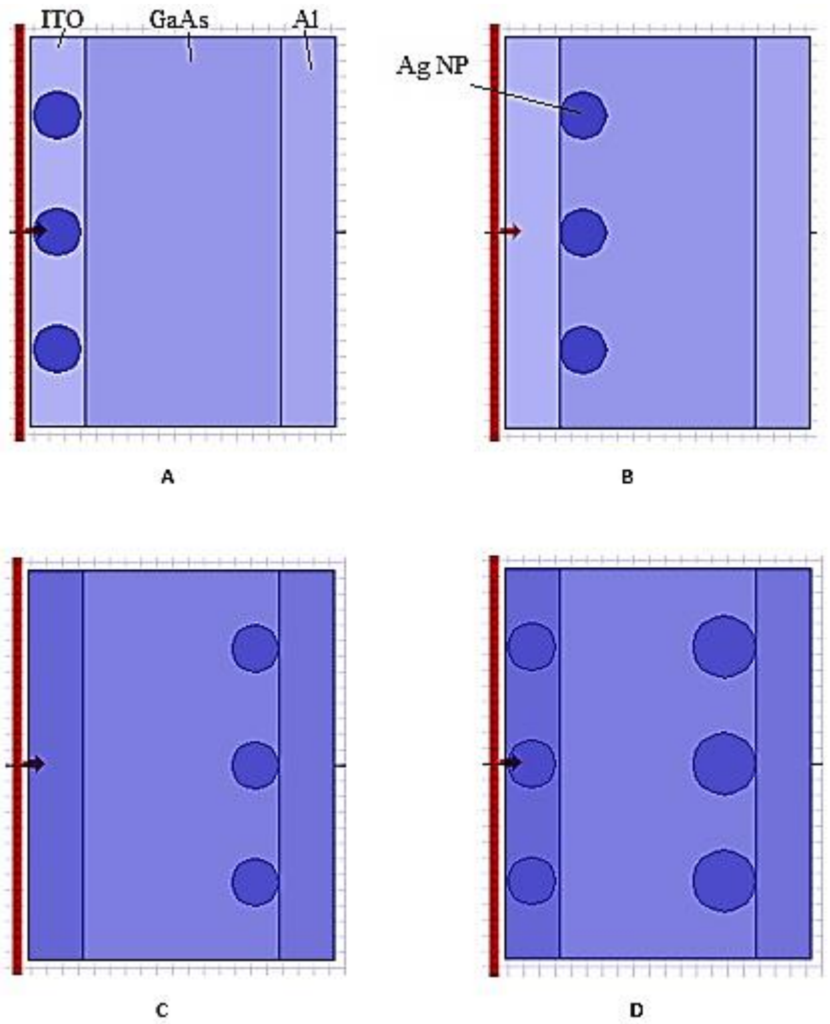


Figure 5.7 Four different structures having NPs at different positions: an Ag NPs with radius 30 nm (A) at the ITO layer, (B) at the top of the GaAs layer, (C) at the bottom of the GaAs layer, (D) at the ITO layer and with a radius of 40 nm at the bottom of GaAs layer.

We observed the following graphs by simulating the structures and get the value of the power spectrum of reflectance at the centered wavelength 600 nm.which is listed below in the table.

Table 3. The power spectrum of Reflectance for different positions of Ag nanoparticles.

Nanoparticle position	The power spectrum of Reflectance (W/m)
A	2.18
B	1.9
C	1.42
D	0.38

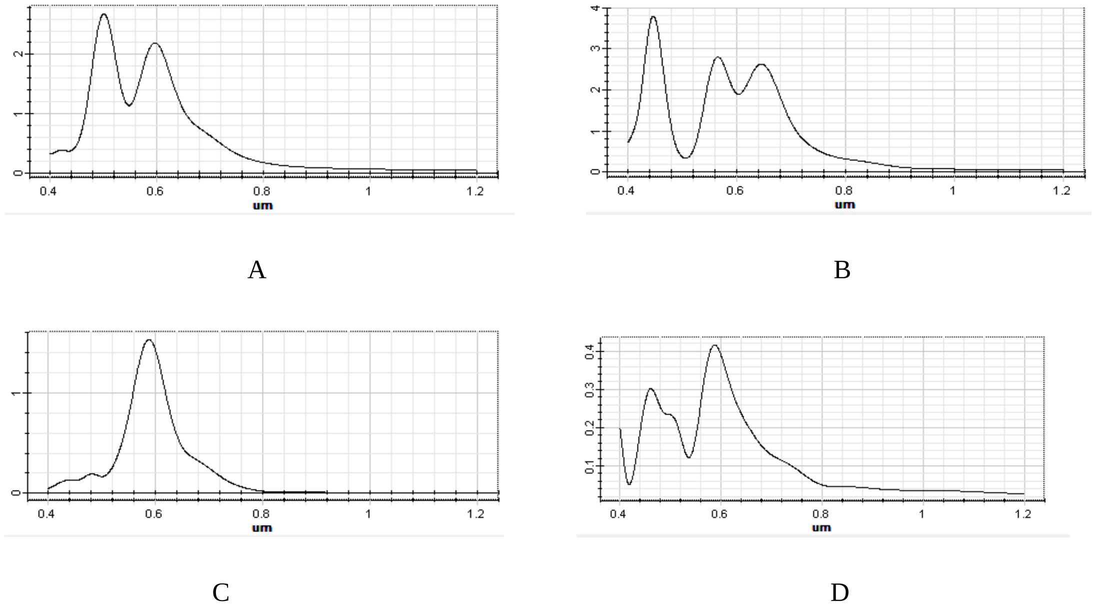


Figure 5.8 Simulation results of four different structures having NPs at different positions:a Ag NPs with radius 30 nm (A) at the ITO layer, (B) at the top of the GaAs layer, (C) at the bottom of the GaAs layer, (D) at the ITO layer and with a radius of 40 nm at the bottom of GaAs layer.

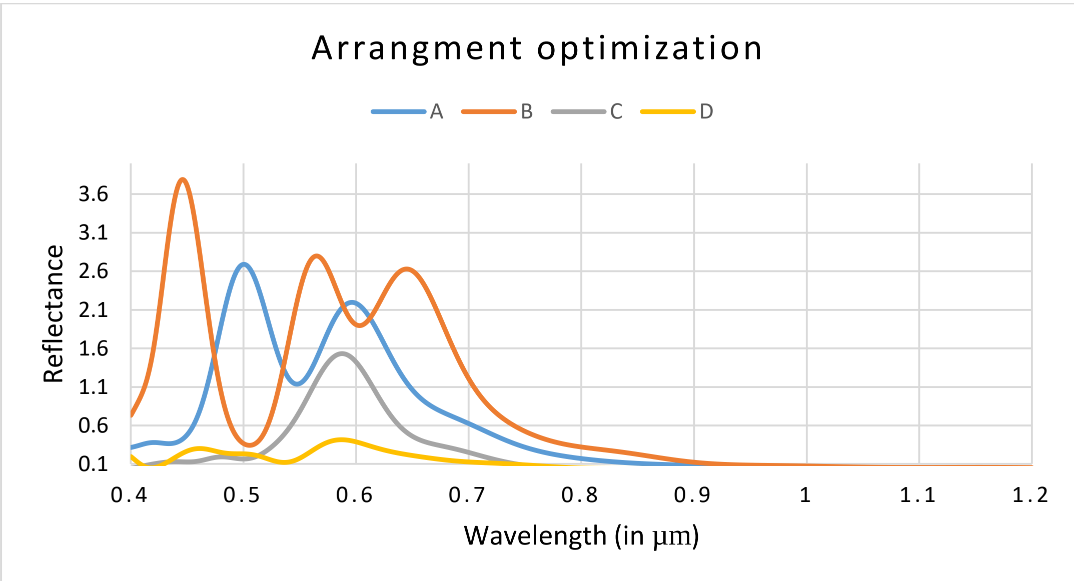


Figure 5.9 Comparison of the power spectrum of reflectance for different positions of Ag nanoparticles.

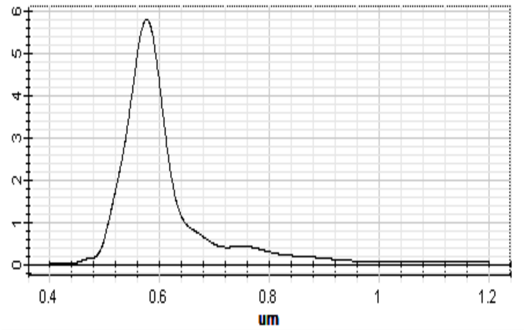
By comparing the graph A, B, C, we have concluded that around the visible region of the EM spectrum. Only structure A and C showed a minimum reflectance than the B structure. The Range of wavelength is from 550 nm to 750 nm and above it also. So we have introduced the D structure which is the combination of A and C. while combining these two, we have increased the radius of the NPs in C structure from 30 nm to 40 nm just because of the ample space in GaAs layer and also knowing the fact that with an increase in size, reflectance decreases.

Thus the structure D show very less reflectance than the others in the desired wavelength range and region. It is shown in the above figure. Besides reflectance and absorption, transmittance also occurs in the structure. So now we look at the power spectrum of transmittance.

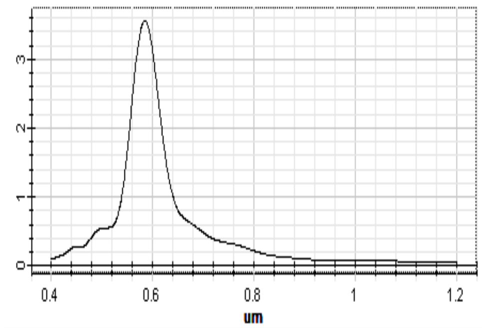
5.3 Transmittance through the structure

5.3.1 Material Optimization

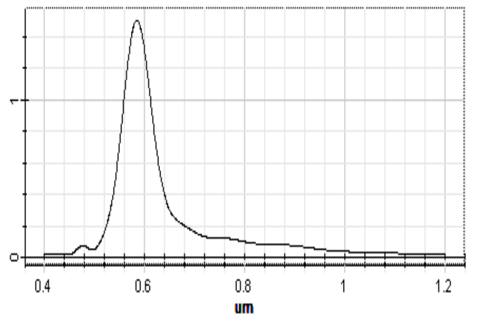
Below are the observed graphs on the optical line 2 where there should be minimum transmittance of light from passing through the structure. These graphs are between the power spectrums of transmittance versus wavelength, for different materials like Al, Ag, Au, and Cu and also with no NP.



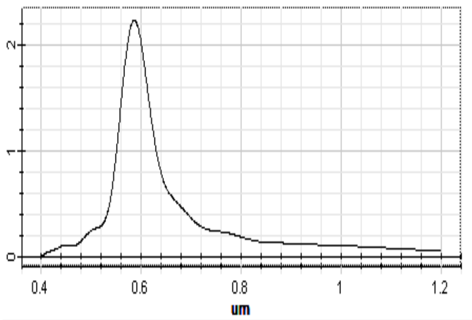
No NP



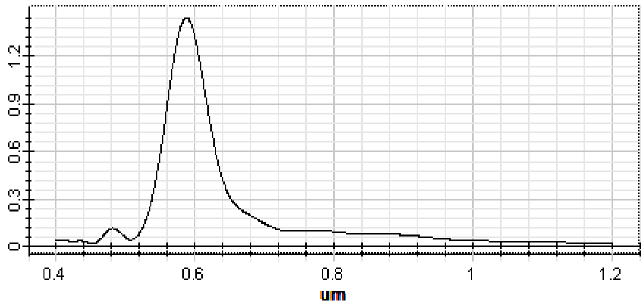
Cu NP



Au NP



Al NP



Ag NP

Figure 5.10 Transmittance versus wavelength graph for the structure with different embedded nanoparticles.

At centered wavelength 600 nm, they show different values as shown below in the table.

Table 4. The power spectrum of Transmittance of different metal nanoparticles.

Metal Nanoparticle	The power spectrum of transmittance (W/m)
No NP	4.2
Al	2.01
Ag	1.21
Cu	3.10
Au	1.2

Now, if we combine all the graphs for comparison .then it will be like the below figure. In this, we observed that when no NP is embedded in the structure, it shows the maximum peak of transmittance between the wavelength ranges of 550 nm to 650 nm. Then followed by Cu NP and Al NP. Then minimum transmittance is shown by Gold (Au) and silver (Ag) nanoparticle. Where Ag NPs shows the minimum value in the 550 nm to 600 nm range and after that, they overlap with each other. Hence, Ag NP embedded in the ITO layer show minimum transmittance in the visible region of the EM spectrum. It can conclude that the better choice to maximize the coupling efficiency of the active layer is via using silver NP.

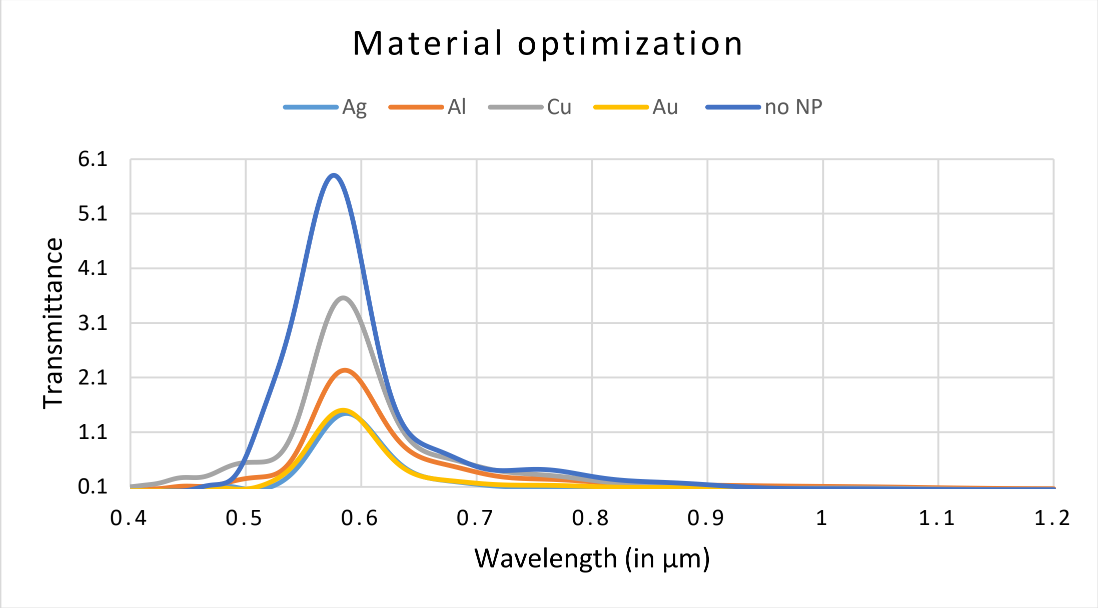
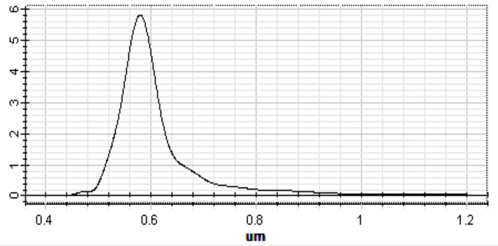


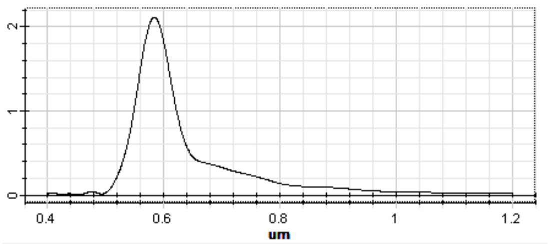
Figure 5.11 Comparison of the power spectrum of transmittance for different nanoparticles.

5.3.2. Size Optimization

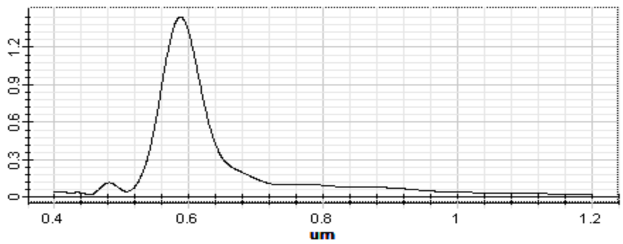
Here we analyze the transmittance characteristics for different sizes of optimized nanoparticle i.e. Ag (silver). We observe different graphs of reflectance for different sizes that are 10nm, 20nm, and 30nm. Below are the graphs,



10 nm



20 nm



30 nm

Figure 5.12 Transmittance versus wavelength graph for the structure with different sizes of Ag NPs.

At centered wavelength 600 nm, they show different values as shown in the table.

Table 5. The power spectrum of transmittance for different sizes of Ag nanoparticle.

Nanoparticle radius (in nm)	The power spectrum of transmittance (W/m)
10	4.54
20	1.81
30	1.41

It can be concluded from the table that with an increase in the size, transmittance decreases and we can't increase the size above 30 nm as the ITO layer is 70 nm thick. Below is the comparison graph of a different plot of different sizes of NP.

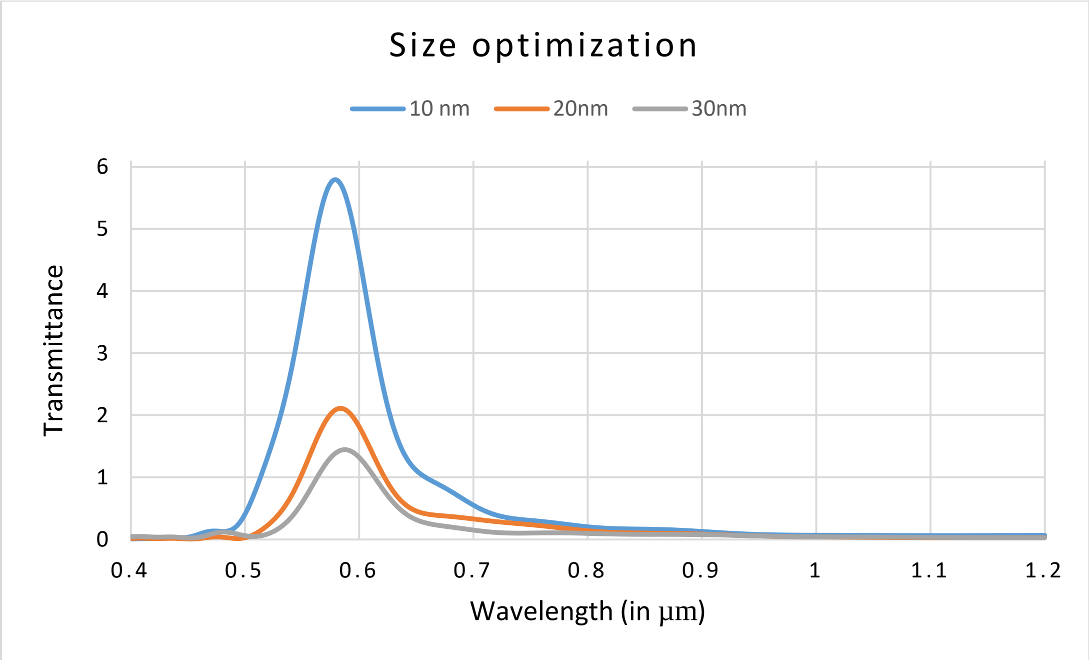


Figure 5.13 Comparison of the power spectrum of transmittance for different sizes of Ag nanoparticle.

Here it can be observed that between the wavelength ranges of 550 nm to 800 nm, Ag NP with the 30 nm radius has a very low level compared with others. Also, it can be said that minimum transmittance is observed in the visible region. That means more absorption of solar radiance can occur because of the low transmission. So the structure is optimized with the Ag NPs with 30 nm radius.

5.3.3. Arrangement Optimization

After material and size optimization, the position of Ag NPs are arranged at four different locations as shown in the figure. First, all three NPs at a definite period are arranged in the ITO layer. The structure which is used for the above two optimizations.

Then, they have been positioned at the top of the Gallium Arsenide (GaAs) layer with equal spacing and radius nearer to the ITO layer. After finding the results, we again change the position of NPs, by placing them at the bottom of the GaAs layer and at last, by observing these different positioned structures, we have placed them in the ITO layer and as well as at the bottom of the GaAs layer. But now their radius is different, in the GaAs layer we have not the limitations of as such had in the Ito layer.

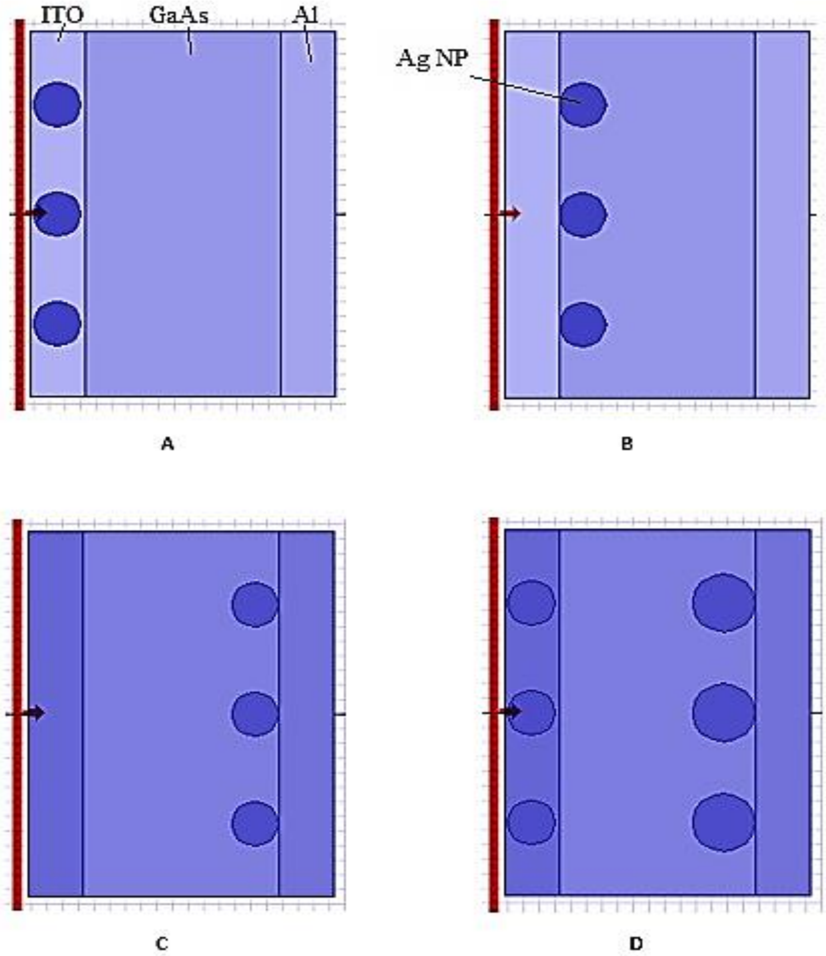


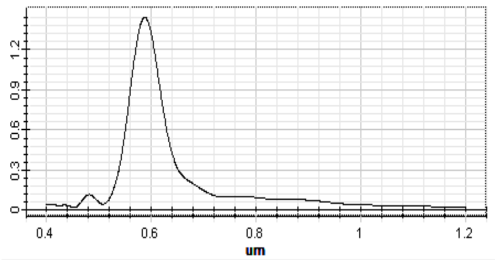
Figure 5.14 Four different structures having NPs at different positions: an Ag NPs with radius 30 nm (A) at the ITO layer, (B) at the top of the GaAs layer, (C) at the bottom of the GaAs layer, (D) at the ITO layer and with a radius of 40 nm at the bottom of GaAs layer.

We observed the following graphs by simulating the structures and get the value of the power spectrum of transmittance at the centered wavelength 600 nm.which is listed below in the table.

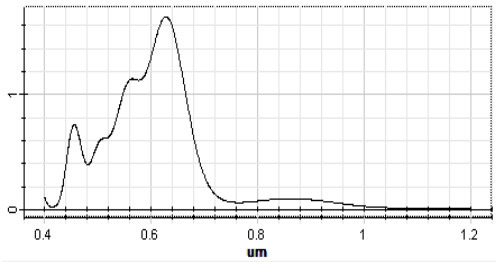
Table 6. The power spectrum of Transmittance for different positions of Ag nanoparticles.

Nanoparticle position	The power spectrum of transmittance (W/m)
A	1.41
B	1.32
C	1.12
D	0.25

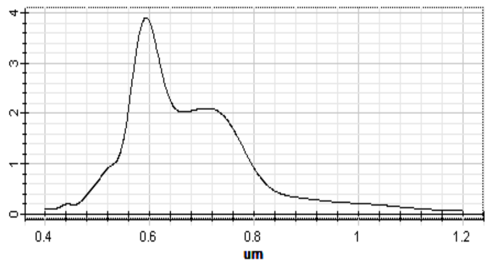
Following are the exactly observed graph from the Optifdtd software simulator for the different structures that have been shown above in the figure.



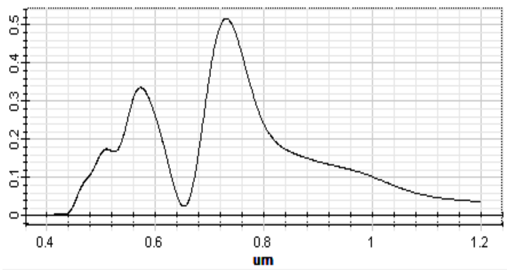
A



B



C



D

Figure 5.15 Simulation results of four different structures having NPs at different positions: a Ag NPs with radius 30 nm (A) at the ITO layer, (B) at the top of the GaAs layer, (C) at the bottom of the GaAs layer, (D) at the ITO layer and with a radius of 40 nm at the bottom of GaAs layer.

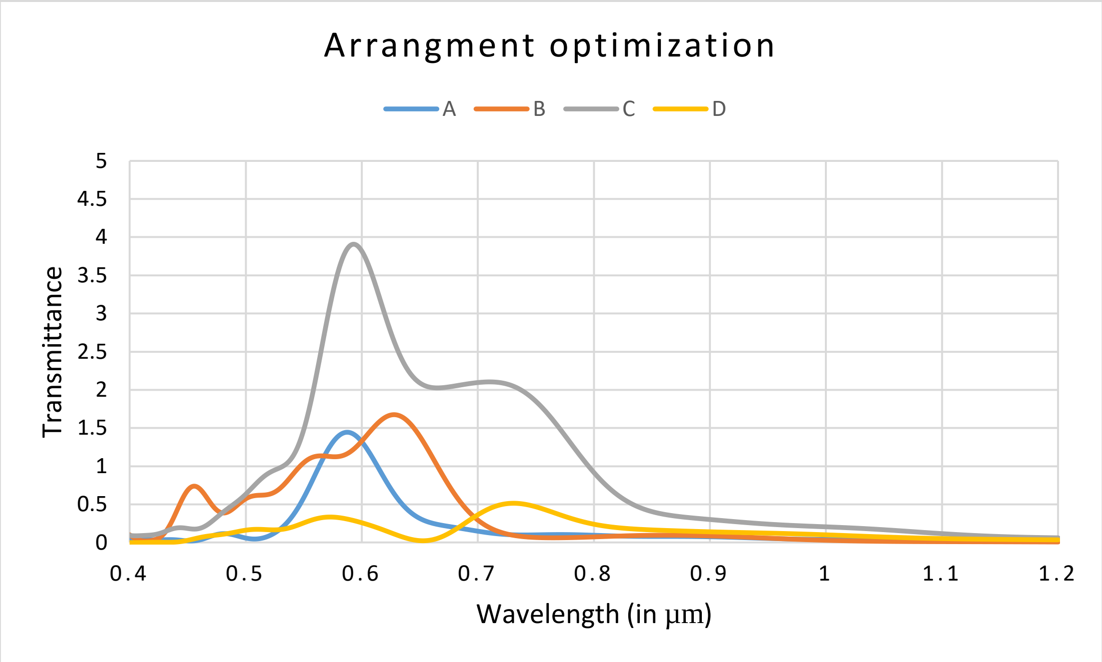


Figure 5.16 Comparison of power spectrum of transmittance for different positions of Ag NPs.

By comparing the graph A, B, C, we have concluded that around the visible region of the EM spectrum. Only structure A and C showed a minimum reflectance than the B structure. The Range of wavelength is from 500 nm to 750 nm and above it also. So we have introduced the D structure which is the combination of A and C. while combining these two, we have increased the radius of the NPs in C structure from 30 nm to 40 nm just because of the ample space in GaAs layer and also knowing the previous result that with increase in size, transmittance decreases.

Thus the structure D show very less transmittance of solar light through it, than the others in desired wavelength range and region. It is shown in the above figure.

Hence our optimized structure is D.

5.4 Electric field analysis of the optimized structure

The optimized structure is having six nanoparticles of Silver (Ag) metal in which three NPs with radius 30 nm positioned at ITO layer and other three NPs with radius 40 nm placed at the bottom of the GaAs layer. After the simulation, we observe the electric field (Ey) result which is shown below,

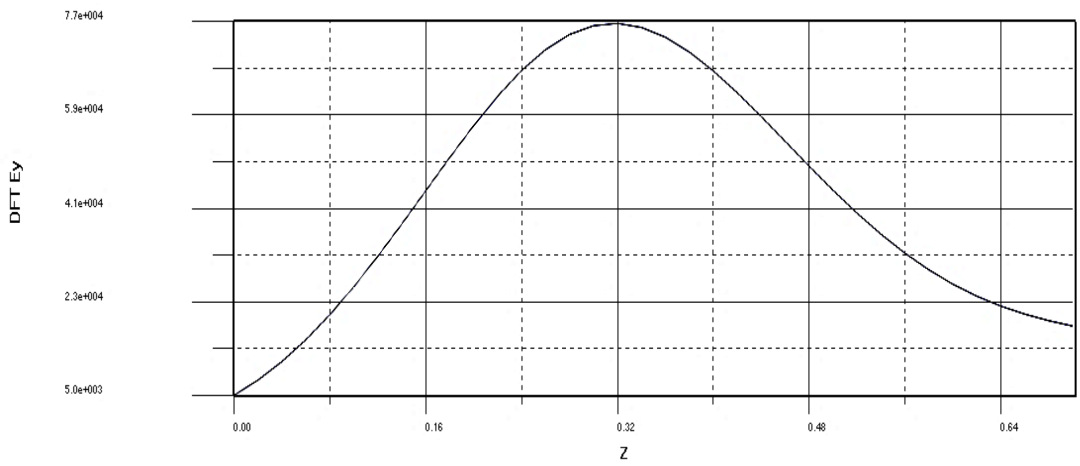


Figure 5.17 2-D graph of Electric field (Ey) across the optimized structure.

From the above figure, it can be observed that the maximum peak of the electric field (Ey) for structure in the X-Z plane at 0.32 µm. Our structure lies on the scale of z-axis around 0.16 µm to 0.48 µm and this is the propagation axis of incident wave.

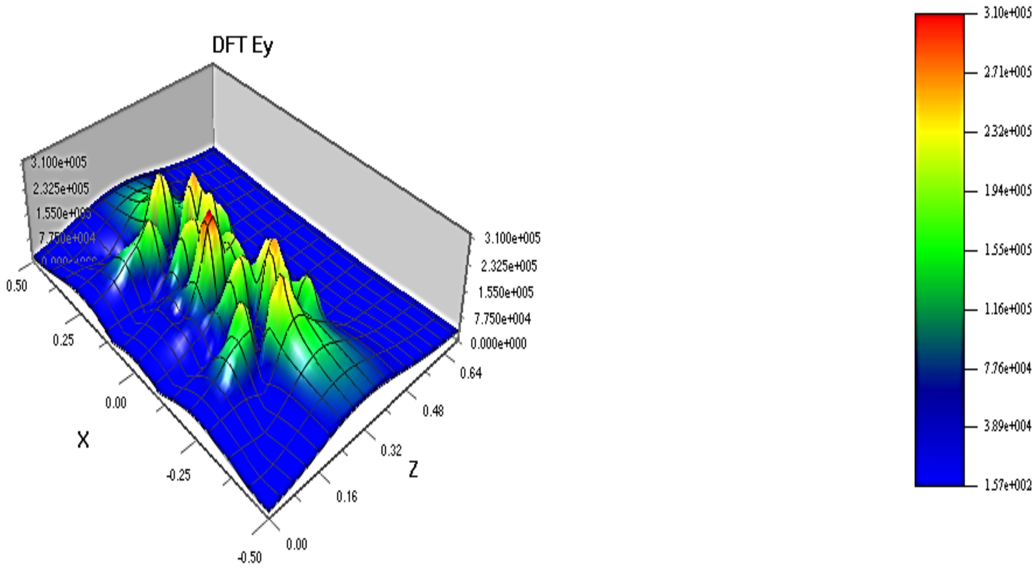


Figure 5.18 3-D diagram of the Electric field (Ey) across the optimized structure.

We can also observe different peaks in the 3-d plot of the electric field. This shows that more and more light is being trapped inside the active layer Gallium Arsenide and more absorbance of light is there.

Now let’s look at the 2-d and 3-d plot of the structure with **no NP** in it.

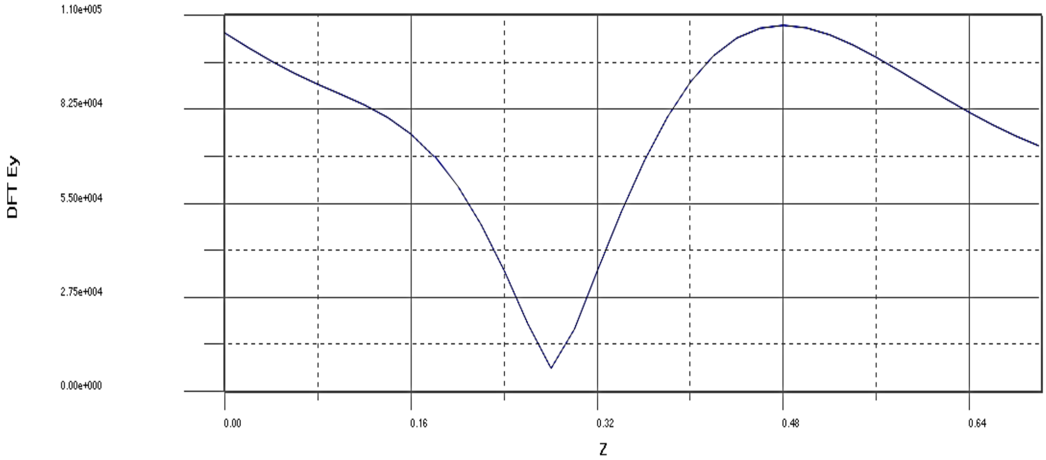


Figure 5.19 2-D graph of Electric field (Ey) across the structure having no NP.

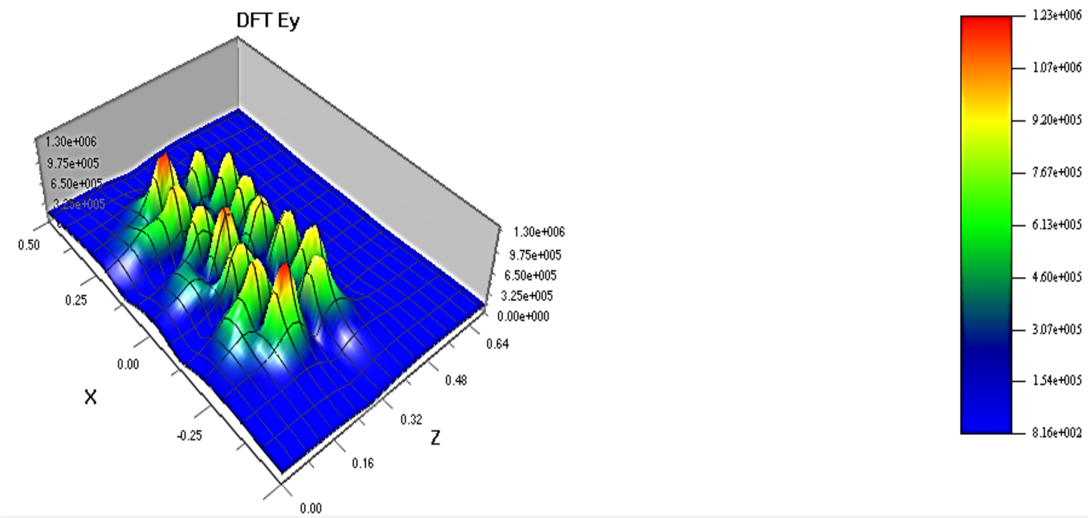


Figure 5.20 3-D diagram of Electric field (Ey) across the structure having no NP.

From the above plots, it can be observed that a sharp low level is found at between the 0.16 µm and 0.32 µm. That same is observed in the 3-d plot of the structure. It means that light is not trapped in the active layer precisely.

5.5 Efficiency of the Optimized Structure

The optimized structure is designed again in the R-Soft software, as it has a tool to compute the solar cell's efficiency. We have designed the exact structure with the same number of nanoparticles with the same radius as defined in the previous section. After using the solar utility, following the J-V curve are observed. That is when No NP is used in the structure and the other one is when optimized structure with NP is used.

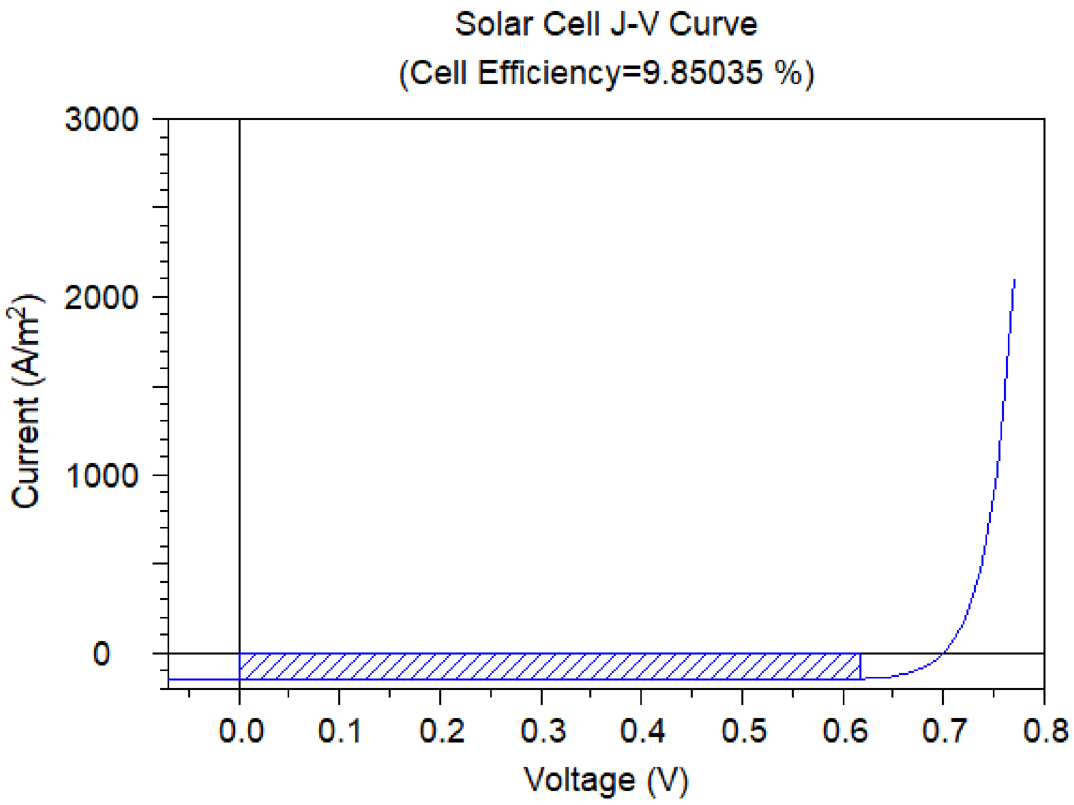


Figure 5.21 J-V curve of the structure with no NP embedded in it.

We get the cell efficiency, η = 9.85 % for this structure. Now for the structure having six nanoparticles is shown below.

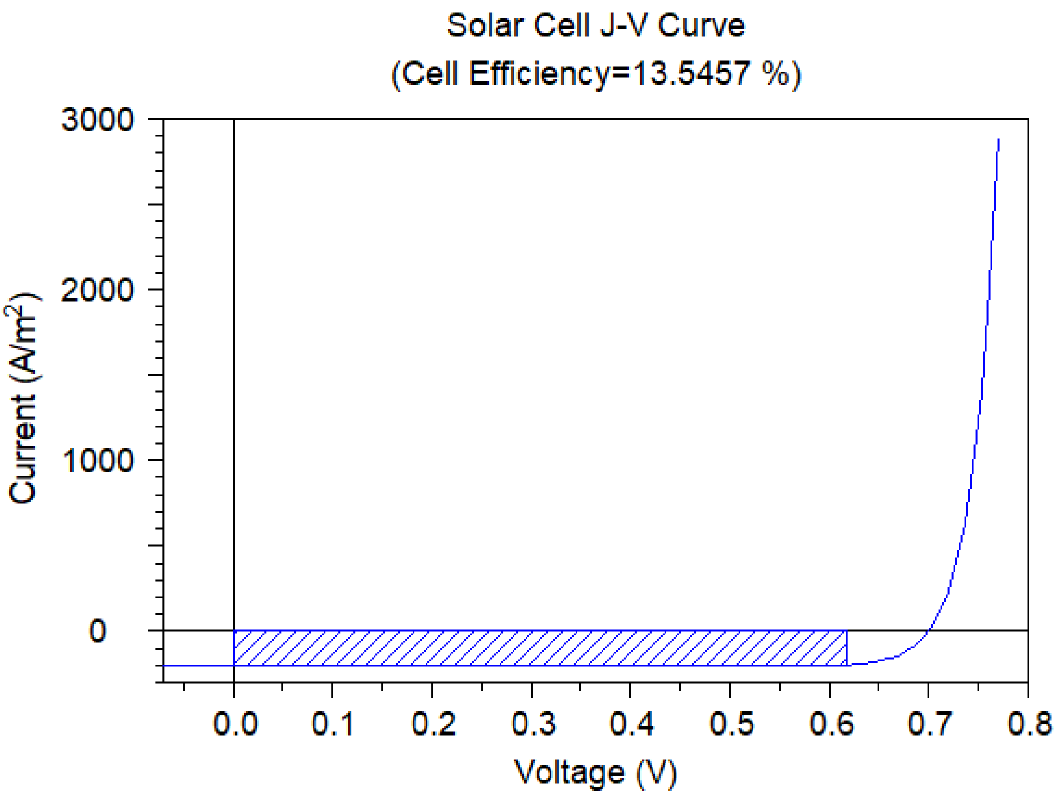


Figure 5.22 J-V curve of the optimized structure.

Here, we get the cell efficiency, η = 13.54 % for this optimized structure. Hence we observe around 4 % increment in the efficiency of the solar cell.

Chapter 6. Conclusion and future scope

Our motive is to couple the thin films with the Nanoparticles such that it can be useful for solar applications. For that, we have optimized the structure via varying the materials of the Nanoparticles, by increasing their size and lastly by rearranging them to yield the optimized structure. To enhance the absorption values in the active layer, we tend to minimize the reflectance and transmittance across the structure.

In material optimization, we have varied the material of the nanoparticles. And we concluded that the copper nanoparticle shows maximum reflectance and transmittance from the front face of the solar cell, followed by the aluminum nanoparticle. But for the silver and gold nanoparticle, they show less reflectance and transmittance across the visible and infrared region, where maximum solar irradiance is also there. So they are the best option for the metal nanoparticles. And silver gives the optimum result than others and moreover, these nanoparticles scatter more of the incident light in the active layer due to plasmonic effects.

In size optimization, by fixing the material of the nanoparticles. We have been increasing the radius of the metal nanoparticles from 10 nm to 30 nm and observed that there is a decrement in the reflectance and transmittance values. This shows with an increase in the radius there is an increase in the absorption value.

In arrangement optimization, we have to change the positions of the nanoparticles for three positions in the structure itself. Then by observing their reflectance and transmittance graph, we have designed a composite structure of it. That structure shows the minimum reflectance and transmittance compare to others. Hence it concludes that there is more absorption occur in that structure. We concluded that around the visible region where there is most of the solar irradiance energy is there, their absorption is being enhanced by minimizing the reflectance and transmittance and that range of wavelength is around 550 nm to 750 nm. This can also be proved by showing the electric field enhancement in the active layer. We have also compared the solar cell efficiency of structure with no NPs in it with that of Optimized structure and we observe the increment of 4 % of efficiency in the solar cell structure.

So, metal nanoparticles with the thin films solar cell have a great scope in the future as the problem of light trapping and absorption in them can be eliminated easily.

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