Light Trapping Optimization in GaAs Thin Film Solar Cell Using Al Nanoparticles

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Declaration of Authorship

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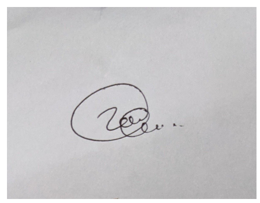

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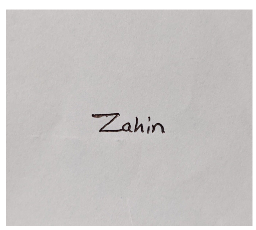

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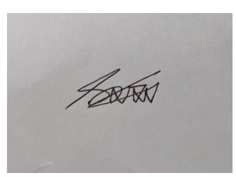

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List of Acronyms

DBR : Distributed Bragg Reflector

SPP : Surface Plasmon Polariton

SPR : Surface Plasmon Resonance

TFSC : Thin Film Solar Cell

SAR: Spectral Absorption Rate

PCB: Periodic Boundary Condition

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We would like to thank Almighty Allah who helped us to complete this thesis work successfully. We have worked very hard throughout the year to accomplish this work. We are very thankful to our respected supervisor Prof. Dr. Md. Ruhul Amin for his continuous help and support throughout our thesis. Without his help, it would have not been possible for us to complete. We would also like to thank our other honorable teachers, friends and family members for their motivation which helped out in our journey of this thesis work.

Abstract

This thesis investigates the application of nanoparticles in thin film solar cell (TFSC) for enhancement of light trapping within the solar cell. The absorption of light within TFSC was monitored while nanoparticles of varying size and shape were applied within the absorptive layer of the solar cell. While most research involving solar cell has been primarily ben conducted with Si, some group III-V semiconductors such as GaAs remains a promising candidate specially as a direct band gap material. Thus. GaAs was used as the absorptive semiconductor material and Al nanoparticles were embedded within the cell. Two different textures were applied to the nanoparticle surfaces and the impact on light absorption was observed. An investigation was also made into the effect of applying multiple layers of nanoparticles within the absorptive layer rather than the conventional single layer. Through these efforts, we have demonstrated that application of Al nanoparticles in GaAs TFSC is effective for enhancing light absorption. Compared to the spectral absorption rate (SAR) of 0.0993 the bare solar cell with no nanoparticle, we demonstrated SAR of 0.3207 with the application of nanoparticles with smooth texture. It was observed that 80 nm radius nanoparticles placed at the top of the absorptive layer was optimal. SAR of 0.3267 and 0.3355 was obtained when a rectangular and triangular textures were given to the surface of the nanoparticles. Furthermore, with the application of multiple layers of nanoparticles, the SAR obtained was 0.5780 was obtained. These results clearly demonstrate that application of multiple layers of nanoparticles and also adding texture to those nanoparticles is effective for enhancing light trapping within the solar cell.

These works have been done via the use of Comsol Multiphysics software. Different models were created to test the various types of nanoparticle's impact on the absorption of light and a comparison between the different models has been presented. The simulations were carried out for light of wavelength varying from 400 nm to 1250 nm. This choice of wavelength range is due to the fact that solar radiation in this range is the most intense and thus most relevant for practical application of solar cells. The SAR for all the models were calculated for the mentioned wavelength range and used to compare between the models.

Chapter 1

Introduction

1.1 Background

Currently, most of the energy demand of the world is met by the use of fossil fuels like oil, natural gas and coal. Fossil fuels are formed as a result of animal decomposition and plant remnants containing carbon. In the year 2019, roughly 84% of the global energy demand was bet by fossil fuels. A major impediment to the continued use of these sources of energy is their limited minable years [1]. Fossil fuels fall under the category of non-renewable energy, i.e. they do not replenish themselves within human timescale. But, the global energy consumption is predicted to keep increasing rapidly [2]. Thus fossil fuel being the major source of global energy supply is a cause for concern. Due to the increase in energy consumption, according to current trends, the consumption of fossil fuels will rise exponentially. Thus, the possibility of running the earth's fossil fuel resources dry is real and has to be dealt with as soon as possible. Otherwise an energy crisis is imminent. Table 1.1 shows that still the overwhelming majority of the global energy consumption comes from nonrenewable sources like oil, gas and coal.

Table 1.1: Analysis of global energy consumption from different sources in 2019 [3]

Energy source	Consumption (exajoules)	Annual change (exajoules)	Share of primary energy	Percentage point change in share from 2018
Oil	193.0	1.6	33.1%	-0.2%
Gas	141.5	2.8	24.2%	0.2%
Coal	157.9	-0.9	27.0%	-0.5%
Renewables	29.0	3.2	5.0%	0.5%
Hydro	37.6	0.3	6.4%	0.0%
Nuclear	24.9	0.8	4.3%	
Total	583.9	7.7		

In addition to the finite and diminishing nature of fossil fuels, their impact on the environment has to be taken into account as well. These sources of energy contribute to the emission of carbon dioxide and other greenhouse gases and are one of the primary causes for global warming. The greenhouse gases are also responsible for atmosphere pollution and respiratory problems in humans.

Due to these concerns related to energy crisis and environment, it has become a priority to search for other forms of energy that are more environment friendly and more sustainable. To move to a more sustainable approach to meeting our energy demands, there is a gradual move towards the use of renewable energy sources. The use of hydro, wind, solar power alongside many other forms of energy such as nuclear energy are starting to grow year by year.

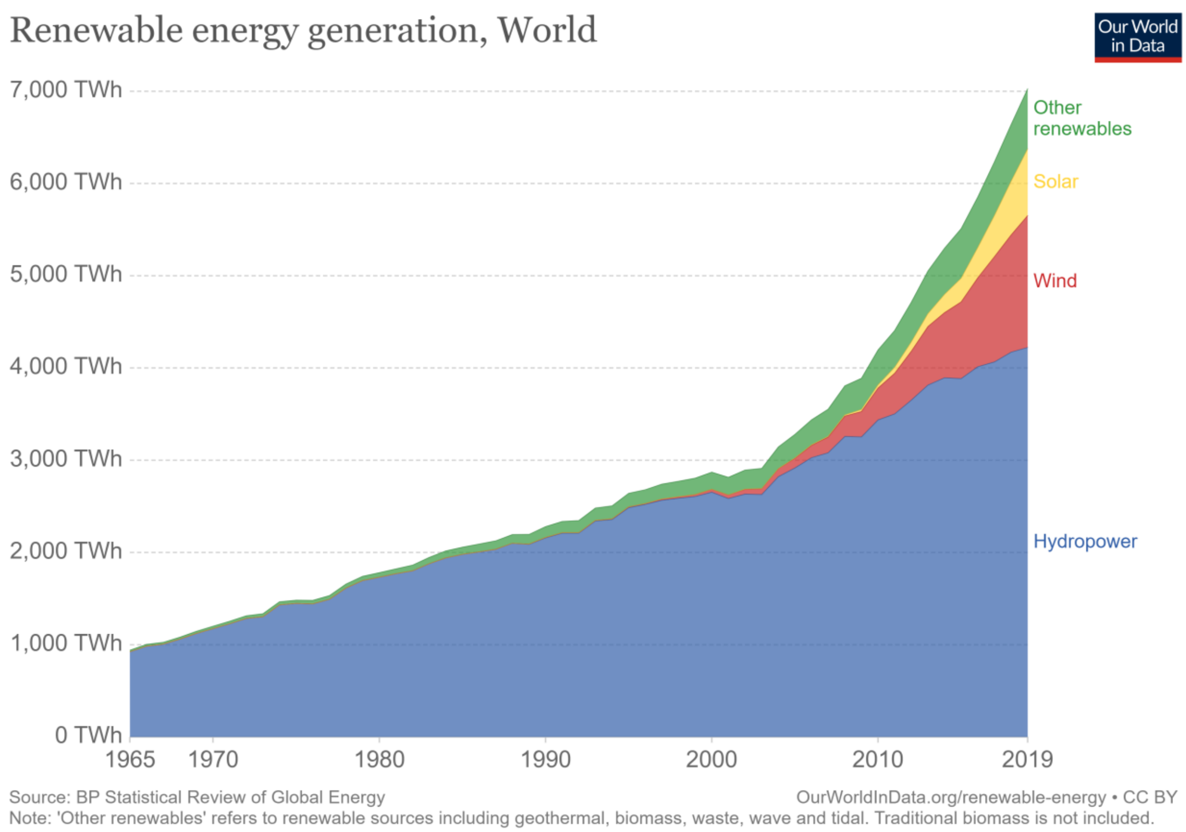

Figure 1.1: The global energy consumption from different sources from 1965 to 2019 [3]

Figure 1.1 demonstrates the exponential growth in the use of different renewable energies worldwide in the several decades. These sources of power not only solve the problem of continued supply, but also has the benefit of being clean and thus favorable for the environment. With global warming and climate change a looming concern for humanity, there is a serious push for moving towards renewable energy sources.

1.2 Solar Energy

Among the alternative forms of energy, hydro, solar and nuclear energy are the most prominent ones. Nuclear energy is one of the leading contenders for possible solutions for this demand. Although nuclear is a possible route, it has the following drawbacks-

- Expensive to construct and maintain.
- Risk of accidents is relatively high compared to other forms of energy.
- Nuclear waste has to be treated and dumped with much caution as any accidents may be catastrophic.

Therefore, to truly have a sustainable approach to meeting our energy demand we must rely on the renewable forms of energy. The performance of solar energy has been particularly prominent. The energy of the sun has been harnessed by humans for thousands of years. But, with the invention of photovoltaic energy in 1954, a whole new dimension of possibilities was opened. Through the use of photovoltaic technology the possibility of supplying energy to the masses utilizing solar energy has become a possibility. This technology primarily uses semiconductor materials to absorb the solar energy and effectively convert that into electrical energy. By the year 2050, photovoltaic energy is expected to cover more than 20% share of the global demand of electricity [4]. In recent years, multiple high conversion efficiencies of silicon solar cells have been reported [5]. This makes the improvement of solar cell efficiencies a very promising goal for the foreseeable future.

1.2.1 Structure and Working Principle

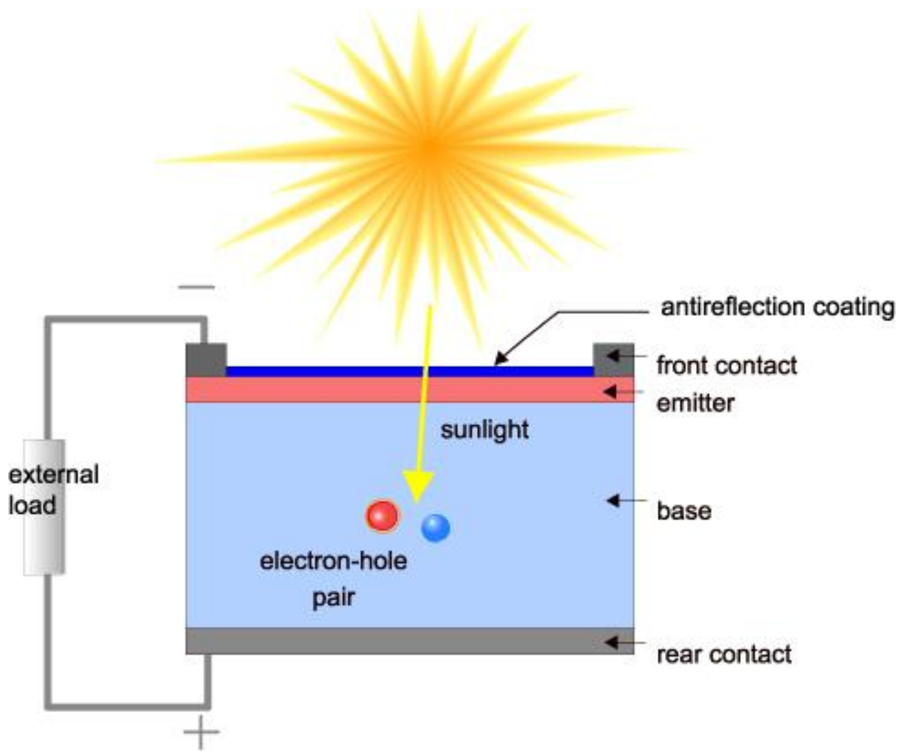

Figure 1.2: Basic Structure of a Solar Cell

Figure 1.2 depicts the basic functionality of a solar cell. It effectively acts as a photodiode. When light falls on the cell, it creates electron-hole pairs within the cell which in turn can flow through the front and read contacts to produce electricity.

Solar cell technology has provided a promising area of investigation for harnessing the energy of the sun. Crystalline silicon, for example has proven to be very effective both in the laboratory and in commercial integration, and comprises of up to 90% of the global market[6].The pros and cons of the use of solar energy has been highlighted in Table 1.2.

1.2.2 Advantages and Disadvantages of Solar Energy

Table 1.2 highlights some of the advantages and disadvantages of the use of solar energy.

Table 1.2: Advantages and disadvantages of solar energy

Advantages	*Disadvantages*
• No fuel required.	• Sunlight has a relatively low energy density.
• .No waste generated. Thus, no contribution to global warming.	• Installation cost of solar panel is high.
• No moving parts. So wear and tear to the equipment is incurred.	• No efficient energy storage system.
• High reliability (>20 years)	• Dependent on sunlight. Solar energy not obtained at night.
• Very safe	
• Quick installation	
• Can be integrated into various types of building structures.	

1.2.3 Classification of Solar Cell

Solar cells can broadly be classified into two categories namely wafer based and thin film solar cell (TFSC). But other than these two, there are some recently emerging solar cells technologies that show promise. Among them, dye-sensitized solar cell, perovskite solar cell and quantum dot (QD) solar cell are mentionable.

Figure 1.3 is a tree diagram showing the categorization of different kinds of solar cell technologies.

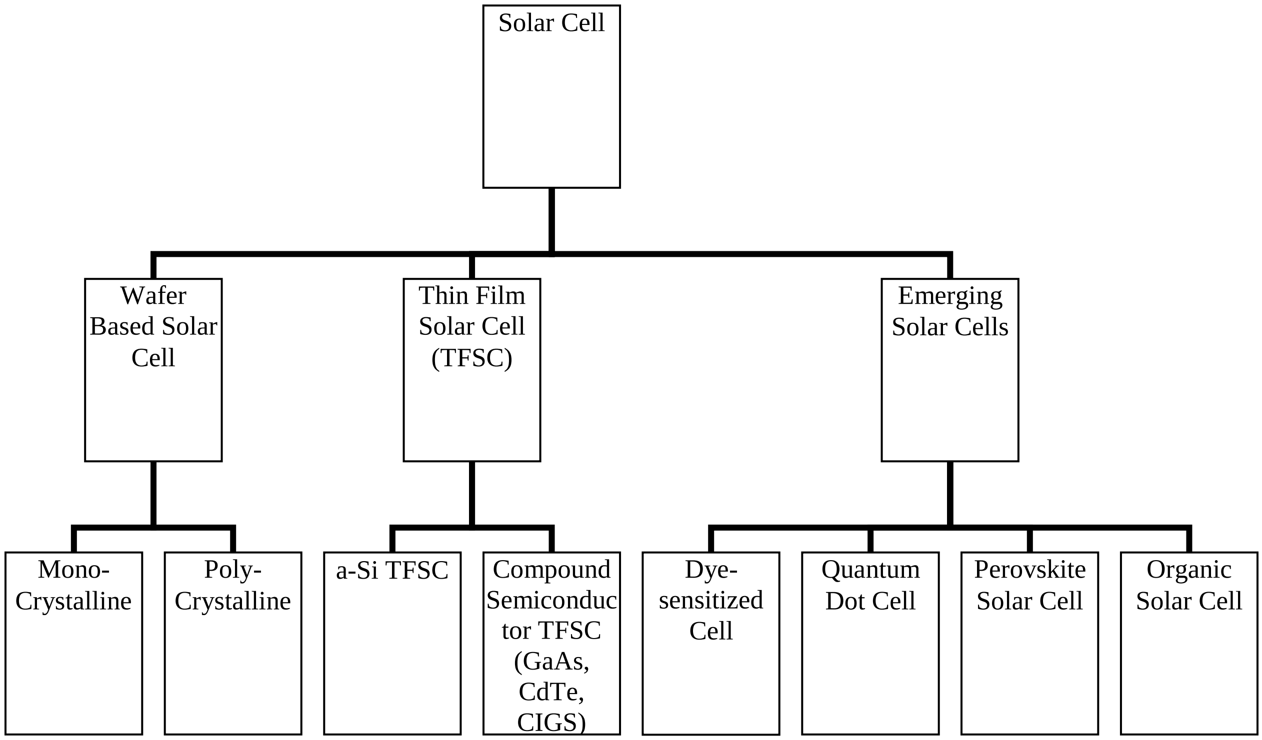

Figure 1.3: Classification of Solar Cells

1.2.4 History of Photovoltaic Cells

The photovoltaic effect is the generation of electron-hole pairs in semiconductor material then light is incident on them. This effect was first observed by French physicist A. E. Becquerel in 1839. But the invention of the first photovoltaic cell came many years later. Charles Fritts created the first photovoltaic cell in 1883 with efficiency less than 1%. The first practical photovoltaic cell was however developed at Bell Laboratories in 1954 by three scientists- Daryl Chapin, Cavlin Souther Fuller and Gerald Pearson [7]. They achieved an efficiency of 6% using a silicon p-n junction.

Throughout the years, many different technologies regarding photovoltaics have been developed. From the 1970s to the start of the 2000s, several technology such as thin film solar cell, multi-junction solar cells etc. have been introduced. In recent years, there have been dye-sensitized cells, perovskite cells and quantum dot solar cells have been introduced. Today solar cells have become a technology commonly known by everyone.

1.2.5 Silicon or III-V Materials

Most of the research regarding solar cells have been focused on using silicon. But, fundamentally Si is not a very appropriate choice for absorbing solar radiation. Firstly, it is an indirect band gap material, which makes absorption of radiation quite an inefficient process. Secondly, it's band gap is lower than what would be optimum for terrestrial application. Thirdly, Si has a lower absorption coefficient than other semiconductor materials.

III-V compounds like on the other hand have some advantage over Si. GaAs is a direct band gap material which makes it more suitable for absorption of light. It has a more appropriate band gap of 1.424 eV. Furthermore it has a higher absorption coefficient, electron mobility and minority carrier lifetime than Si.

1.2.6 The Need for Thin Film Solar Cells

While crystalline silicon solar cells have proven to be an effective way to obtain high efficiencies, they are not very cost effective in terms of material usage. For solar cells to have high penetration in the market, it needs to excel at efficiency while simultaneously minimizing material cost. To provide for the world's energy needs without minimization of the requirement of semiconductor material is not feasible. Therefore, a need for new technology has been created to minimize the material requirements of solar cells. Thin film solar cells (TFSC) have been proposed for solving this problem. Some of the advantages of TFSC are as follows-

- Require less semiconductor material. Allowing for scalable production.
- Lower cost of production allowing for scalable production.
- Requires low processing temperature.
- Can be produced on flexible substrate.

1.2.7 Light Trapping in Thin Film Solar Cell (TFSC)

To deal with this problem of material cost and availability, thin film solar cells (TFSC) have been used. Reducing the thickness and therefore the material amount of the absorber layer can be very useful for decreasing the high production cost. Till now, most of the established PV technologies are based on crystalline silicon and around 10% of the productions rely on thin-film technologies. Typically TFSC have thickness of order of a few micrometers (~1µm) which is two orders of magnitude less than that of regular solar cell (~100µm). This cuts down on the material cost by a very large extent. But this creates a new problem. The thickness of the cell being so small, allows for light to escape the cell without much time spent within the cell, causing very poor absorption of power within the cell.

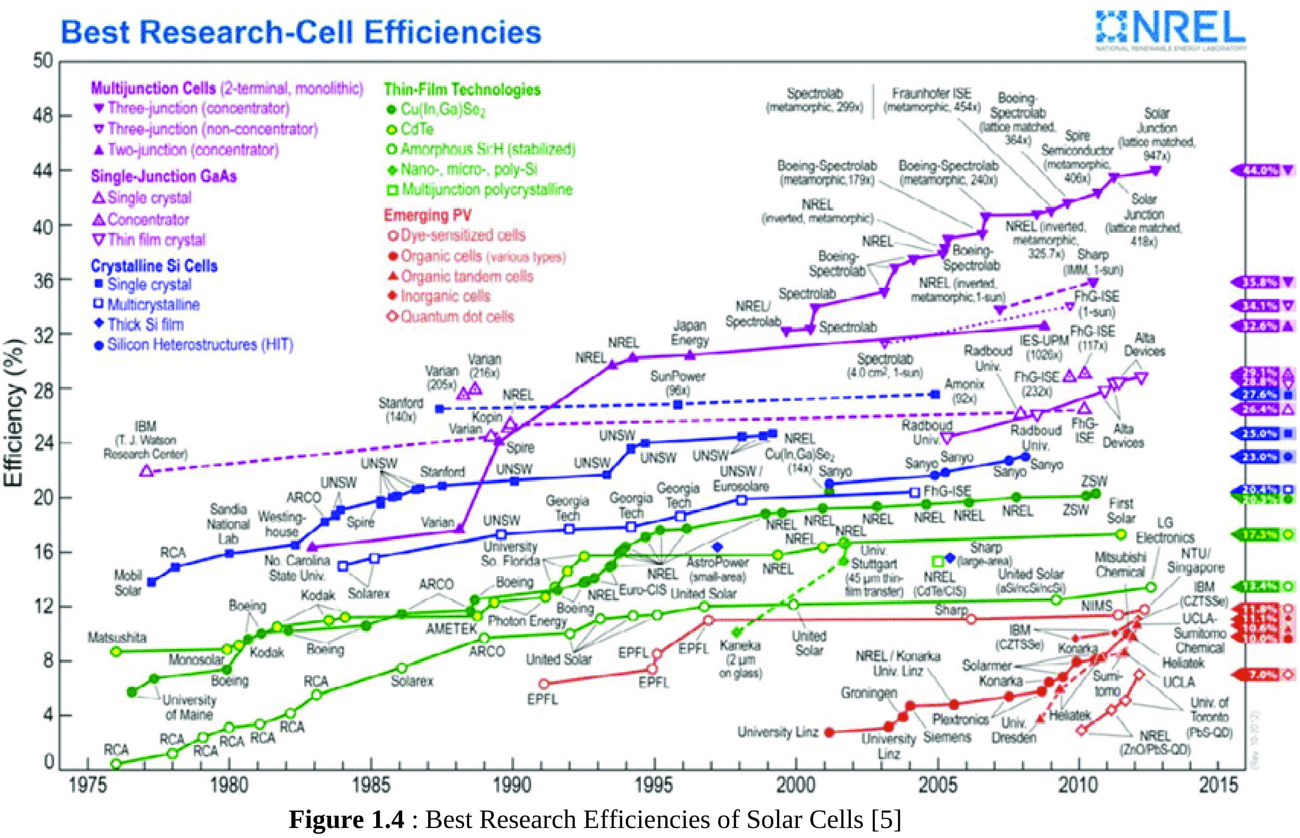

Figure 1.4 : Best Research Efficiencies of Solar Cells [5]

In Figure 1.4 we see that the efficiencies of TFSC is lagging behind that of traditional crystalline solar cells. To combat this, and improve the performance of TFSC various light trapping mechanisms have been proposed. Light trapping refers to techniques used for artificially elongating the optical path length of light within the solar cell so that the overall absorption within the cell is improved. One of the more promising approaches is the application of nanostructures within the absorptive layer of the cell [8-11].

1.3 Problem Statement

Thin film solar cells have been around since the 1970s. They provide a solution to one of the most fundamental problems with using solar power on a large scale, which is the problem of production cost and material availability. TFSC aims to reduce the sheer amount of semiconductor material needed by reducing the thickness of the solar cell. But, this creates problems of its own. Due to the thin nature of TFSC, the light absorption within the cell is very inefficient. Thus a simple TFSC fails to make good use of a large portion of the solar energy incident on it. To solve this problem, the use of light trapping mechanisms such as the use of nanoparticles has been promising. In our work, we aimed to explore this approach for increasing TFSC performance.

1.3.1 Literature Review

Several approaches have been explored to date to solve the light absorption problem in TFSC. Among these approaches, one of the most prominent techniques is to use nanoparticles within the absorptive layer. Nanoparticles have been used to improve the performance of TFSC through three main mechanisms-

1. Light Scattering with nanoparticles at the top surface of the cell.
2. Excitation of SPR by embedding nanoparticles in the semiconductor material.
3. Excitation of SPP by having a metal/semiconductor interface at the rear end.

When a nanoparticle is placed in between two dielectric mediums, light incident on the nanoparticle scatters more in the direction of the medium with greater permittivity. This effect has been leveraged to produce enhancement in TFSC performance. An 8% increase in short circuit current in GaAs solar cell has been reported through the use of Ag nanoparticles at the top surface [8]. Rokeya et al. used finite difference time domain (FDTD) method to place Al and Ag nanoparticles on top of a Si solar cell with Si_3N_4 antireflection coating [9]. They varied the size and shape of the nanoparticles and their periodicity to find out that when optimized, Al nanoparticles performed better than optimized Ag nanoparticles.

The effect of embedded nanoparticles in the absorber layer has also been demonstrated to improve absorption compared to a cell with no nanoparticles [10]. Singh and Verma reported a current density improvement of 50.5% using Al nanoparticles in GaAs TFSC [45]. Noguez et al. demonstrated that the SPR excitation significantly varies with change in size and shape of nanoparticles and their environment. This brings up the need for optimizing the configuration of nanoparticles within the solar cell to get the best possible absorption. Investigation into the effect of manipulating size and spacing of the particles have been carried out [40].

Metal surfaces at the back of the solar cell have been used for exciting SPP in the cells, which effectively turns the direction of propagation of energy by 90º. This greatly increases the optical path length of the solar cell. Several applications of SPP in TFSC have been reported already [47]. Ferry et al.[48] showed 26% short circuit current enhancement and Lee et al.[49] found 41% absorption enhancement through the excitation of SPP in TFSC. SPP has also been explored in GaAs solar cell and 14.2% improvement in short circuit current density has been reported through the application of 6nm Ag film in TFSC where GaAs is the substrate [50].

1.4 Our Objective

In our work, we have made an attempt at observing the effect of applying different types of nanoparticles in the absorptive layer of thin film solar cells on the light absorption within the cell. Due to there being a lack of research focusing on GaAs TFSC, although GaAs is a good candidate for TFSC, we have decided to use it as the semiconductor of choice in our work. The goal was to monitor the effect the nanoparticles would have on the light absorption within the cell and also to see how the variation of the dimensions, position and material of the nanoparticles affect the absorption of light. We applied nanoparticles with several types of textured surfaces to the TFSC to observe their effect on light absorption. Using Comsol Multiphysics, we developed several models with GaAs as the substrate, with a Ag back reflector and Al nanoparticles of varying radius inserted at varying positions throughout the cell. Through this process, we also aimed at finding the optimal particle dimension and position. Our objectives are summarized as-

- To observe effect on absorption using nanoparticles with varying textures.
- To observe the effect of varying the position of the nanoparticles within the absorptive layer.
- To find an optimal size of nanoparticles for absorbing solar radiation.
- To find an optimal position of the nanoparticles within the solar cell.

1.5 Organization of the Thesis

This text has been divided into six chapters. The first chapter explains the current situation of energy demands in the world and the role solar energy plays in it. Also, the need for TFSC has been introduced here and an explanation of our objectives in this thesis has been provided.

The second chapter dives into the different approaches that have been applied to improve light trapping within TFSC. It describes the different methods such as the application of plasmonic and photonic nanostructures within the cell to improve light trapping.

The third chapter discusses the methodologies we have used for conducting our work. It outlines the simulation software used, the models that we have designed and the mathematical models used for running the simulations. Visual representations of the simulations we have constructed have been provided. Arguments for why we chose the types of models we chose have also been made in this chapter.

Chapter four dives into the results of our work. It shows the different results and the comparison between our work and other results presented in the literature.

Chapter five summarizes the work we have done and suggests future works that can be carried out based on our results.

Chapter 2

Light Trapping Methods in TFSC

2.1 The Need for Light Trapping

The primary impediment to the widespread use of TFSC is the fact that the photon absorption within the absorptive later is very inefficient due to its thin nature. As the light falls on the solar cell, the photons penetrate the cell and pass through it without being absorbed. This is because each photon does not spend nearly enough time within the solar cell to ensure that it is absorbed. Thus most of the light ends up passing right through the solar cell as depicted in Figure 2.1.

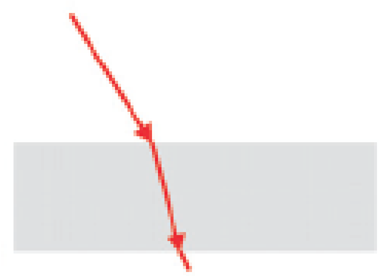

Figure 2.1: Simple TFSC without any light trapping [12]

Back metallic back reflectors have been introduced to reduce the light escaping from the back of the solar cell. This effectively doubles the optical path length of the light within the cell. But this still leaves us with the problem of light escaping from the top surface of the solar cell as shown in Figure 2.2.

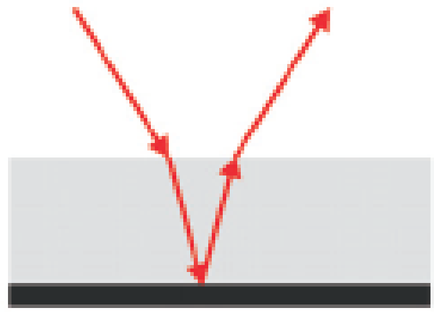

Figure 2.2 : Simple TFSC with metallic back reflector [12**]**

To ensure efficient use of photons incident on a TFSC, various light trapping mechanisms other than a simple back reflector have been applied. These mechanisms essentially have the purpose of trapping the photons incident on the TFSC in the absorptive layer which increases the likelihood of each photon being absorbed. Once the photons are in the absorptive region of the cell, it is necessary for the photons to spend enough time in that region to be absorbed. But, for most semiconductor materials, the absorption coefficient decreases rapidly for increasing wavelength of light, meaning that the light needs to spend more time in the absorptive layer to be absorbed.

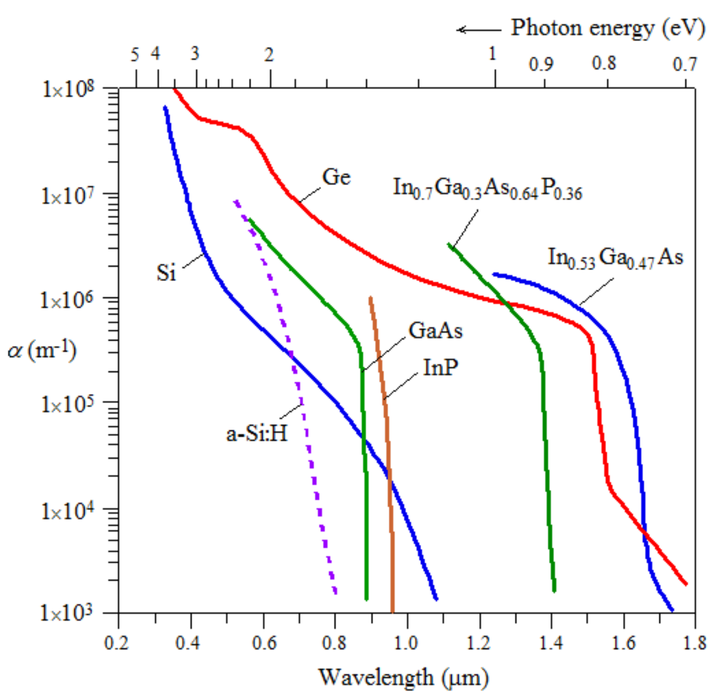

Figure 2.3: Absorption Coefficient vs Wavelength of commonly used Semiconductor materials

From Figure 2.3, we see that for both Si and GaAs the absorption coefficient is much smaller than that required for good absorption for most of the solar spectrum. The situation is particularly dire for the case of the higher wavelengths. Thus, a large number photons that enter a TFSC would pass through it without being absorbed. This leads to extremely poor efficiency.

To solve this issue of light absorption in the cell, different mechanisms have been proposed for trapping photons in the absorptive layer long enough for most photons to be absorbed. The main purpose of light trapping techniques are threefold. They are-

- Decrease incident light reflection
- Increase the light absorption
- Modify the optical response of the device for use in different applications

While many unique methods have been applied up to now to improve light trapping in solar cell, the following approaches have been used most commonly and to very good effect.

- Photonic Nanostructures
- Periodic Grating Structures
- Random Scattering Surfaces
- Plasmonic Structures

2.2 Photonic Nanostructures

Photonic crystals of various kinds have been used in recent years to manipulate the optical path of photons inside the absorptive layer of TFSC. Most commonly one dimensional photonic crystal back reflectors [13, 14] are used in the back surface to cause total internal reflection which increases the optical path of the photons within the absorptive layer.

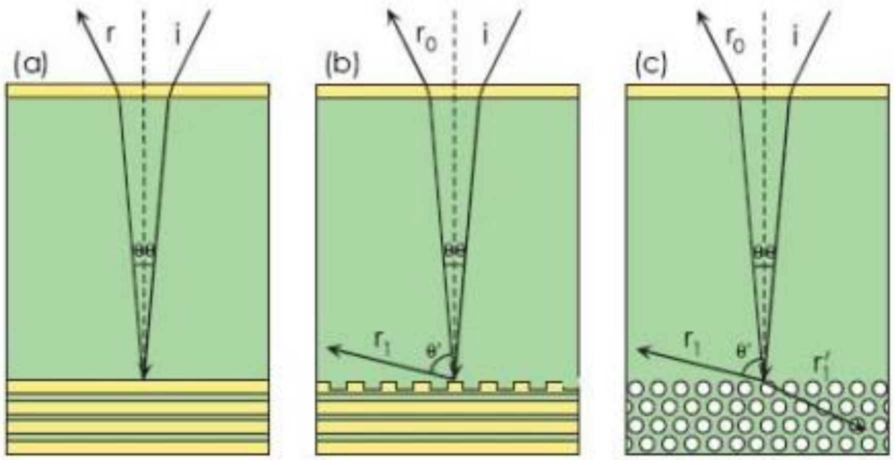

Figure 2.4: Solar cell designs using photonic nanostructures: (a) Distribute Bragg Reflector (DBR) (b) a DBR with a periodically etched grating (c) a photonic crystals [14]

Figure 2.4(a) shows a distributed bragg reflector (DBR) applied to cause total internal reflection within the cell to effectively act as a back reflector. This helps reflect the light without the concern of parasitic losses in case of a metallic back reflector. DBR with grating has been displayed in Figure 2.4(b) where alongside total internal reflection, a scattering effect is obtained as well. The application of photonic crystals is shown in Figure 2.4(c). Two and three dimensional structures have also shown promise. A variety of photonic structures such as nanowires [15], nanocones [16], nanorods [17], nanowells [18], nanopyramids [19], nanopillars [20] and nanospheres [21] have been applied.

2.3 Periodic Grating Structures

Application of periodic gratings is an effective approach [22] to increasing the optical path length within the absorber layer and enhance light absorption within the solar cell. Periodic gratings scatter light that falls on it back into the absorptive region effectively increasing absorption. Through controlling the geometric properties of the grating, such as shape, period, height and duty cycle, one can optimize the performance of the TFSC and also choose the wavelength range where the cell performs best. Application of grating on front and back surface has been shown to significantly improve performance of TFSC [23]. 66.5% improvement in photocurrent through the use of two-dimensional cascaded grating on the top surface with respect to a reference model has been reported [24]. L.Zeng et al. showed improved external efficiency for longer wavelengths with one dimensional periodic grating back reflector [25].

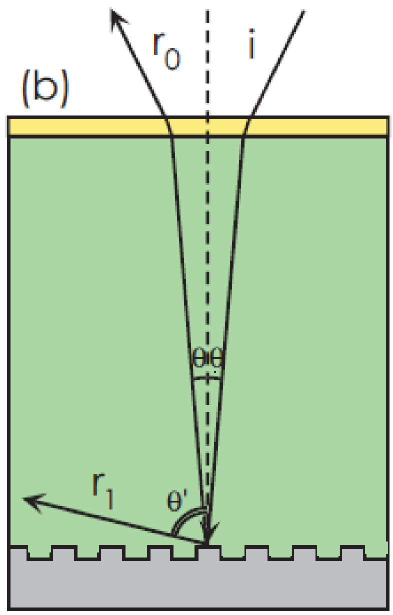

Figure 2.5: TFSC with periodic grating on the back reflector [14]

Figure 2.5 gives an illustration of a simple periodic grating structure applied to a metallic back reflector. The grating causes light scattering at the back of the TFSC and makes the light take an oblique path while travelling back to the top surface which enhances the optical path length, thus leading to better absorption.

2.4 Random Scattering Surfaces

Random scattering surfaces have long been applied to improve the performance of solar cells. Methods such as nanoimprinting [26] and reactive ion etching [27] have been applied to create random scattering surfaces for TFSC. These surfaces effectively increase the absorption of light within the absorptive layer. Textured surfaces with varying haze ratios have been tested to show improvements in performance of TFSC [28].

Figure 2.6 depicts the use of three different textured surfaces applied to the back surface of the solar cell to improve its performance.

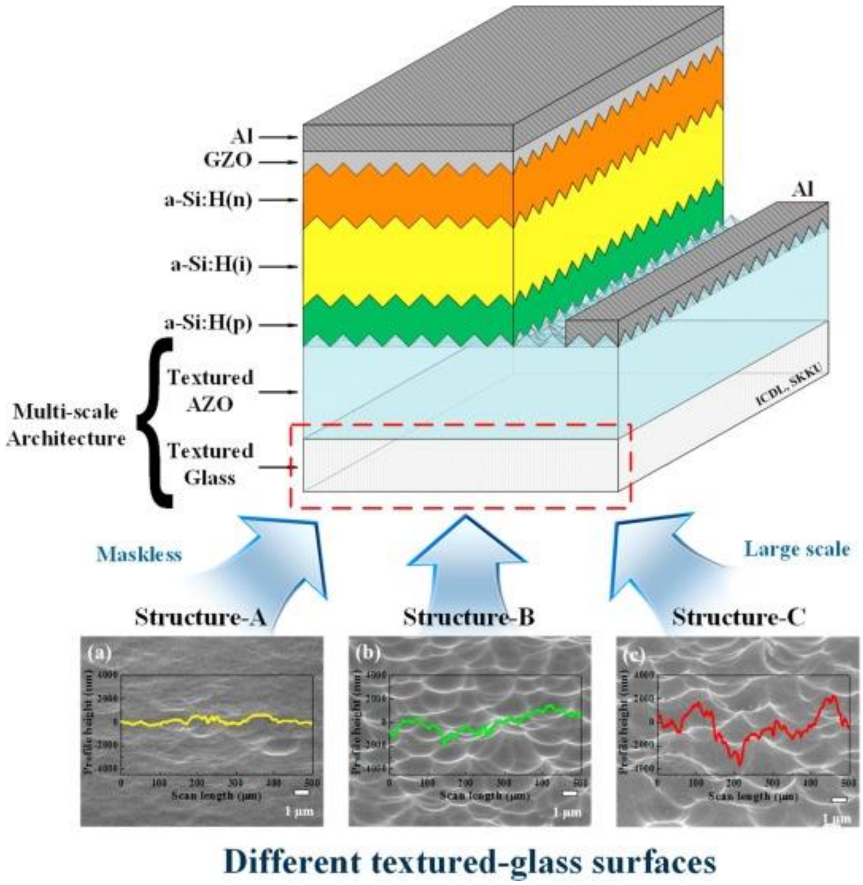

Figure 2.6: Three randomly textured glass structures in amorphous silicon TFSC. [28]

2.5 Plasmonic Structures

Plasmonics is a phenomena that involves interaction between electromagnetic radiation and conductive electrons in metal [29]. Surface plasmons can be excited in essentially two ways. They are exited as either localized surface plasmon resonance (SPR) in metal nanoparticles or as propagating surface plasmon polaritons (SPP) at an interface between a metal and a semiconductor. Significant promise has been shown through the application of plasmonic structures in TFSC [30-32]. Plasmonic structures can be applied in thin film solar cells in primarily three different configurations so that the absorber layer's physical thickness can be maintained in TFSC while increasing the optical thickness.

1. The first of the three configurations places metal nanoparticles the top surface of the absorber layer to scatter the light into multiple directions as it enters the absorber layer.
2. In the second configuration, metal nanoparticles are embedded in the absorber layer. They act as sites for SPR which increases the absorption in the surrounding region.
3. The third scheme has the metal nanoparticles placed on the rear end of the TFSC. They couple propagating light into SPP modes and cause a 90º change in the direction of propagation of light.

2.5.1 Light Scattering Effect

Light scattering is almost symmetrical in both forward and backward directions when the nanoparticles are surrounded by a homogeneous medium [33]. But, the situation changes when the nanoparticles are located in the interface between two dielectric mediums. In this scenario, light scatters more in the direction of the medium with greater permittivity [34]. When light enters the TFSC after being scattered, its optical path length is increased. Furthermore, as some of the light is reflected off the back reflector, some of it can be reradiated into the cell by the nanoparticles at the top. Figure 2.7 shows the scattering effect of nanoparticles placed on top of the solar cell. The optical path takes an angular path instead of a straight one, making the optical path significantly longer and thus improving absorption within the solar cell.

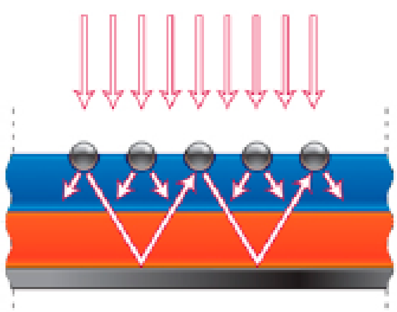

Figure 2.7: Metal nanoparticles placed on the top surface of a TFSC (Scattering) [35]

This phenomenon of improvement of light absorption using resonant scattering was first demonstrated by Stuart and Hall [36, 37]. For wavelengths longer than 600 nm, short circuit current improvement of 8% has been observed in GaAs TFSC using Ag nanoparticles on the top of the absorptive material[38].The behavior of plasmonic nanoparticles depend heavily on their material, size, shape and position.

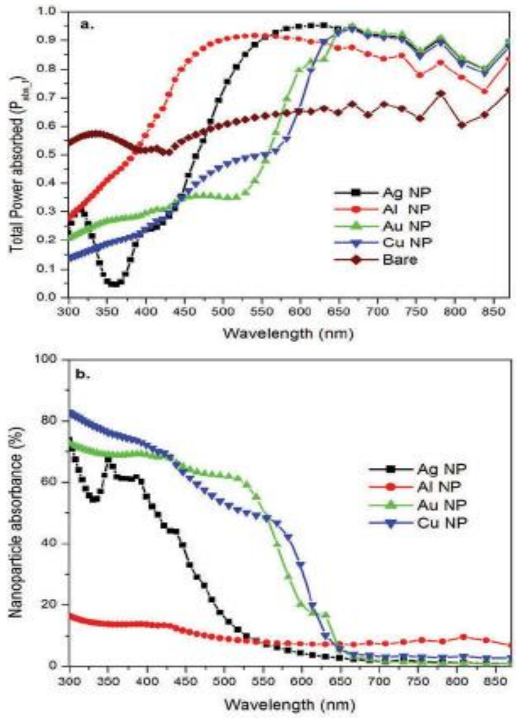

Figure 2.8: Spectral power absorption in GaAs TFSC with optimized metal (Ag, Al, Au and Cu) nanoparticles (a) by GaAs, (b) by metal nanoparticles [39]

The parasitic absorption of Ag and Au particles is quite large at shorter wavelengths. This hinders device performance when these particles are used. But, Al nanoparticles provide significantly less parasitic losses than Ag and Au. Singh and Verma compared the performance of Al, Cu, Ag and Au nanoparticles on the top surface of GaAs TFSC and found that Al nanoparticles gives significantly better enhancement of light absorption than the other tested metals [40].Figure 2.8(a) shows that Al nanoparticles give a greater enhancement of absorption and Figure 2.8(b) shows lower parasitic losses than Ag, Au and Cu.

2.5.2 Surface Plasmon Resonance

When metallic nanoparticles are embedded in the semiconductor material of the solar cell, they act as sites for SPR. When light is incident on the nanoparticles, the energy from the light is stored in the localized SPR. This excitation energy can then be absorbed by the surrounding material through the near-field coupling. This effectively improves light absorption in the solar cell. Small nanoparticles of varying diameter and spacing between nanoparticles have been demonstrated to enhance the plasmonic absorption in solar cells [40,41]. Figure 2.9 demonstrates the excitation of SPR in the metal/semiconductor interface. This allows for greater absorption through the near-field effect around the nanoparticles.

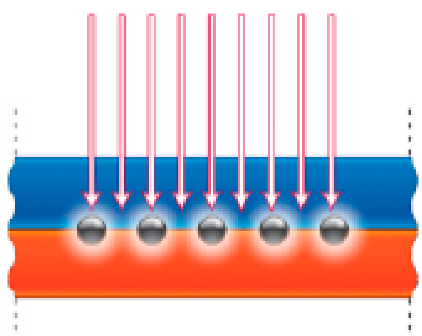

Figure 2.9: Metal nanoparticles embedded in the semiconductor (SPR)[35]

Similar to the case with the light scattering effect, the absorption of light SPR is dependent on the material of the nanoparticles, the spacing between them, their size and shape and the dielectric medium of the absorptive layer [42].

Improved photocurrents due to the plasmonic near-field coupling has been demonstrated for both organic and inorganic solar cells [41, 43]. 5 nm diameter Ag nanoparticle array applied in tandem thin film organic solar cells has been shown to improve absorption [43]. A current density improvement of 50.5% compared to a bare model has been reported by Singn and Verma through the application of Al nanoparticles on top and bottom of GaAs solar cell[45].There have also been investigation into the application of textured nanoparticles instead of simple spherical nanoparticles in solar cells which have shown promise[46].

2.5.3 Surface Plasmon Polariton Modes

Another way in which plasmonic nanoparticles are applied to improve light trapping is through the use of surface plasmon polaritons (SPP). SPP are electromagnetic waves that propagate along the metal/semiconductor interface. The incident light is effectively turned by 90º. This increases the optical path length by several orders of magnitude, thus leading to greater light absorption within the solar cell. The 90º change in the direction of propagation of light in the solar cell because of SPP is demonstrated in Figure 2.10.

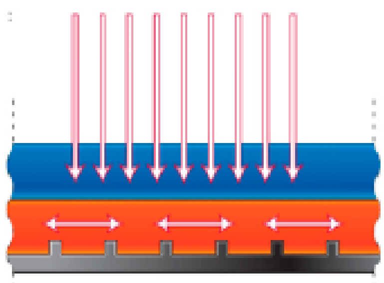

Figure 2.10: Excitation of SPP in TFSC with nanostructured metal films on the back reflector [35]

Several applications of SPP in TFSC have been reported already [47]. Ferry et al.[48] showed 26% short circuit current enhancement and Lee et al.[49] found 41% absorption enhancement through the excitation of SPP in TFSC. SPP has also been explored in GaAs solar cell and 14.2% improvement in short circuit current density has been reported through the application of 6nm Ag film in TFSC where GaAs is the substrate [50].

2.6 Summary

Light trapping is of vital importance if TFSC technology is going to play a significant role in fulfilling the energy demand in the following years. Because of this, it has been a top area of enquiry in recent years. Many different methods have been tried out to find an optimal light trapping approach. Among the many different methods used, the application of nanostructures within the cell has proven itself to be quite effective. Nanoparticles have been incorporated in different ways with TFSC to enhance their performance. Most of the work that has been done has primarily focused on using amorphous silicon as the absorptive layer. Little investigation has been done using theoretically promising materials like GaAs. Thus, we have dedicated our work to applying promising techniques such as the application of nanoparticles in a relatively unexplored material like GaAs.

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Chapter 3

COMSOL Simulation

3.1 Introduction

COMSOL Multiphysics is a cross-platform finite element analysis, solver and multiphysics simulation software. It allows conventional physics-based user interfaces and coupled systems of partial differential equations (PDEs). COMSOL provides an IDE and unified workflow for electrical, mechanical, fluid, acoustics, and chemical applications. The COMSOL Multiphysics software enables the simulation of designs involving coupled physics (EM, mechanics, acoustics, fluid flow, heat transfer, chemical reactions, etc.).

For our research purposes, we have used COMSOL Multiphysics to design the Thin Film Solar Cell (TFSC) structure and apply different variants of embedded nanoparticles in the absorption layer to observe their effect. By varying the position, size and texture of the particles we have generated several sets of data and have calculated different performance parameters.

3.2 Model Setup settings

Space Dimension: 2D

Physics:

Multiphysics

Semiconductor Optoelectronics, Frequency Domain

This is an integration between the two physics *Electromagnetic Waves, Frequency Domain* and *Semiconductor*.

Electromagnetic Waves, Frequency Domain

The Radio Frequency, Electromagnetic Waves, Frequency Domain interface is used to solve for time-harmonic electromagnetic field distributions.

The physics interface supports the study types Frequency Domain, Eigen frequency, Mode Analysis, and Boundary Mode Analysis. The Frequency Domain study type is used for source driven simulations for a single frequency or a sequence of frequencies.

This physics interface solves the time-harmonic wave equation for the electric field.

Semiconductor

The Semiconductor interface solves Poisson's equation for the electric potential and the drift-diffusion equations for electrons and holes in a semiconductor material.

Study:

Frequency-Stationary

The Frequency-Stationary study is used to compute the temperature field, at thermal equilibrium, and the electromagnetic field distribution for models created with the Induction Heating, Microwave Heating, or Laser Heating physics interfaces. It is a special case of a Stationary study where the stationary heat transfer equation is solved together with a frequency-domain equation for electromagnetics.

3.3 Familiarization with Some Parameters Used

L= Wavelength of incident electromagnetic wave

h_t= Height of nanoparticles

r= Radius of nanoparticles

S11= Reflection Coefficient

S21=Transmission Coefficient

P_{abs} =Power absorbed

3.4 Model Geometry

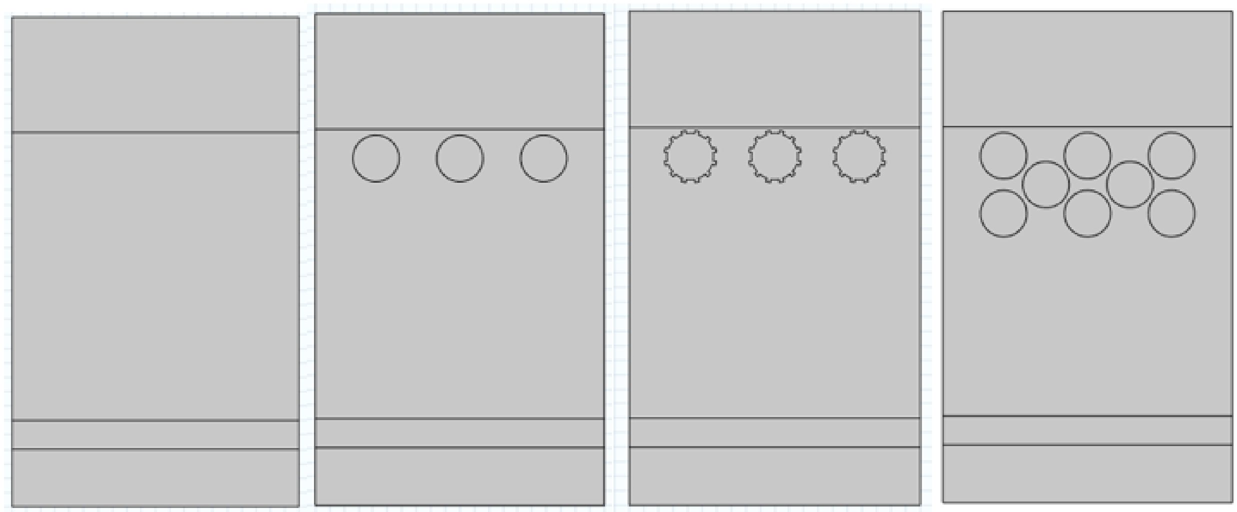


Figure 3.1: Variations in models simulated

Our base model is denoted as the "bare model" (Fig 3.1) and this has been used as a benchmark for comparing to the nanoparticle embedded models with different textures.

The geometry was constructed COMSOL's inbuilt model builder using basic shapes and Boolean operation

3.5 Materials Used

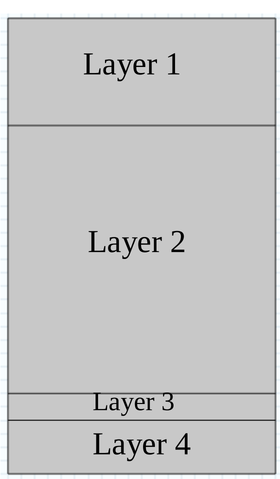


Figure 3.2: Different layers of model being simulated

Layer 1 and 4	Air
Layer 2	Gallium Arsenide
Layer 3	Silver

Aluminum for nanoparticles

Figure 3.2 shows the different layers used in our model. Layer 1 & 4 contains Air. Layer 2 consists of Gallium Arsenide as absorptive layer. The nanoparticles will be embedded within this layer. Layer 3 has silver as reflecting layer. Aluminum was used as the metal for the nanoparticles.

3.5.1 Material Properties

Table 3.1 : Material Properties [51]

Material	Relative permeability	Relative permittivity	Electrical conductivity (S/m)
Air	1	1	0
Aluminum	1	-10.834-1.6505i	3.55×10^{7}
Silver	0.99998	-15.243+0.40284i	6.30×10^{7}

Table 3.2: Semiconductor Properties [51]

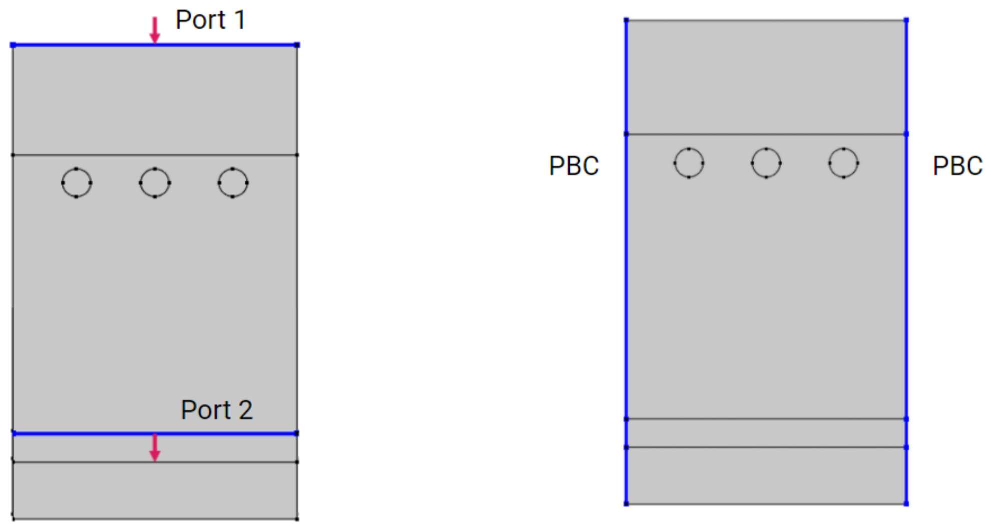
Material	Relative permeability	Relative permittivity	Electrical conductivity (S/m)	Band Gap (V)	Electron affinity (V)	Electron mobility [m²/(V·s)]	Hole mobility [m²/(V·s)]
Gallium Arsenide	1	12.9	1×10^{-6}	1.424	4.07	0.85	0.04

Table 3.1 and Table 3.2 shows the various parameter values that we have used for the different materials to carry out our simulations.

3.6 Model Conditions

Electromagnetic Waves, Frequency Domain

Ports **Periodic Boundary Conditions**



(a) (b)

Figure 3.3: (a) Boundaries selected for ports 1 & 2, (b) Boundaries set up with PBC

Ports are used to provide a path and for measuring the input and output of the electromagnetic waves. Port nodes are placed where electromagnetic energy enters or exits the model. For our model we have selected periodic port as port type (Fig 3.4a). Port 1 was set to have "Wave excitation" as active and Port 2 inactive. Input quantity was "Electric Field" and the electric mode field amplitude for both the ports were x=0 V/m, y=0 V/m, z=1 V/m. The port input power at Port 1 was set at 10W.

Periodic Boundary Condition (PBC) (Fig 3.4b) are a set of boundary conditions that allow for the approximation of a large periodic system by only simulating one unit cell which repeats itself. PBCs allow us to simulate a finite portion of the geometry we are constructing to get results that are transferrable to the whole structure. They allow for the simulation of large structures with limited computational power. In our work, we have only constructed a small portion of the solar cell and placed two PBCs on either side of the geometry to extrapolate our results to an actual solar cell with many repetitions of the created geometry.

3.7 Semiconductor

Analytic Doping

Donor concentration: $1x10^{16}$ [1/cm^3]

Geometric Doping

Acceptor concentration at boundary: $5x10^{18}$[1/cm^3]

Junction Depth: $7x10^{-6}$[m]

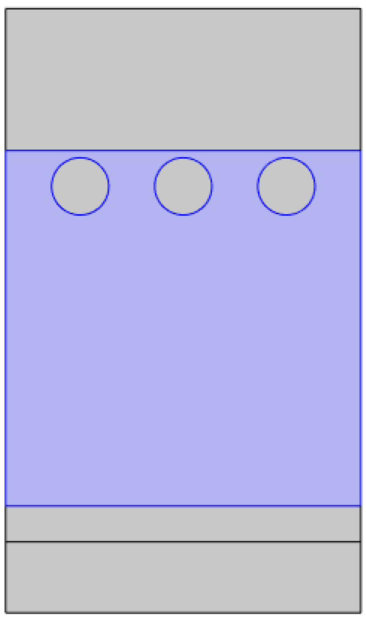


Figure 3.4: Domain selected for Analytic and Trap Assisted recombination

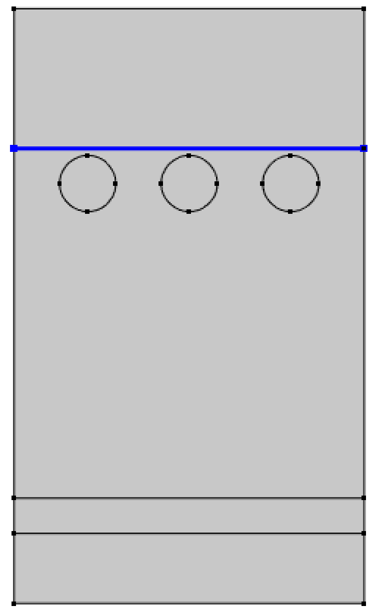


Figure 3.5: Boundary selected for geometric doping

Trap-Assisted Recombination

Trapping model: Shockley Read Hall model

Electron lifetime: $20x10^{-6}$[s]

Hole lifetime: $20x10^{-6}$[s]

3.8 Mesh

Meshing is a very important part of the engineering simulation process. Meshing divides complex geometries into small elements. These elements are used as discrete local approximations all of which together give us the results for the whole structure. A finer mesh provides us with a more detailed results but the simulations become slower with a finer mesh. A coarse mesh on the other hand gives quick result, but the simulation might not converge.

Through-out the structure “fine” mesh was applied with meshing being intensified to “extremely fine” in the absorptive layer around the nanoparticles (Fig 3.7).

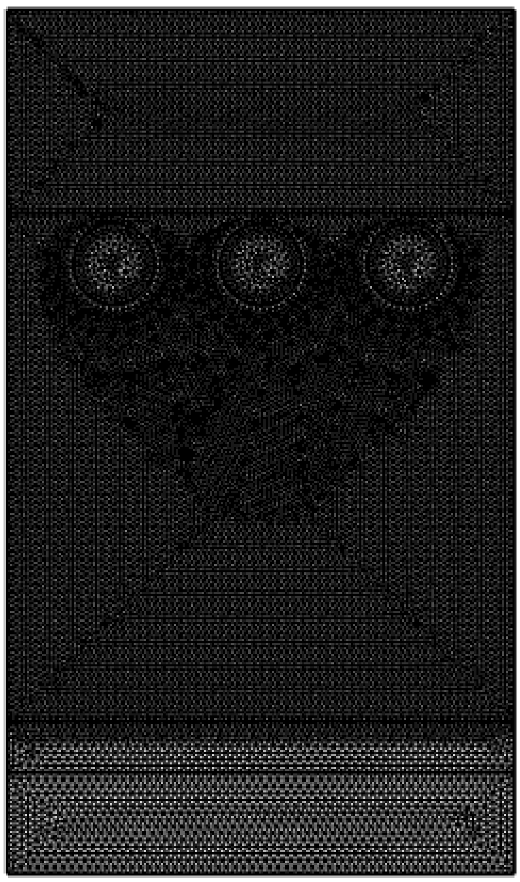
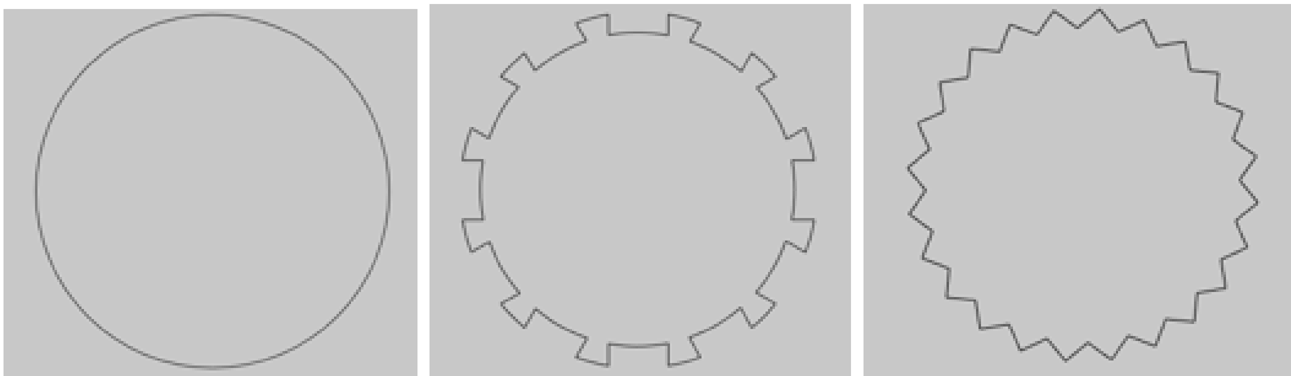


Figure 3.6: Meshed geometry

3.9 Texture of Nanoparticles



(a) (b) (c)

Figure 3.7: (a) Smooth, (b) Rectangular, (c) Triangular Nanoparticles

From M. Vijayalakshmi [46] we have learned about how using textured nanoparticles can improve absorption. There were textures made up of basic cutouts and we've used the idea to come up with more textures and simulated TFSC model for 3 types of nanoparticle texture (Fig 3.8); Smooth, Rectangular and Triangular.

These were embedded within the absorptive layer and simulated at different heights and radii.

3.10 Model Simulation Parameters

3.10.1 Parametric Sweep Range

Majority of the energy of the Sun at sea level exists between 400nm and 1250nm, so we ran our frequency sweep simulation for our TFSC models from 240THz to 750THz (Fig 3.9).

For simplicity we have used wavelength as sweeping parameter and the resolution of steps in the sweep was 10nm.

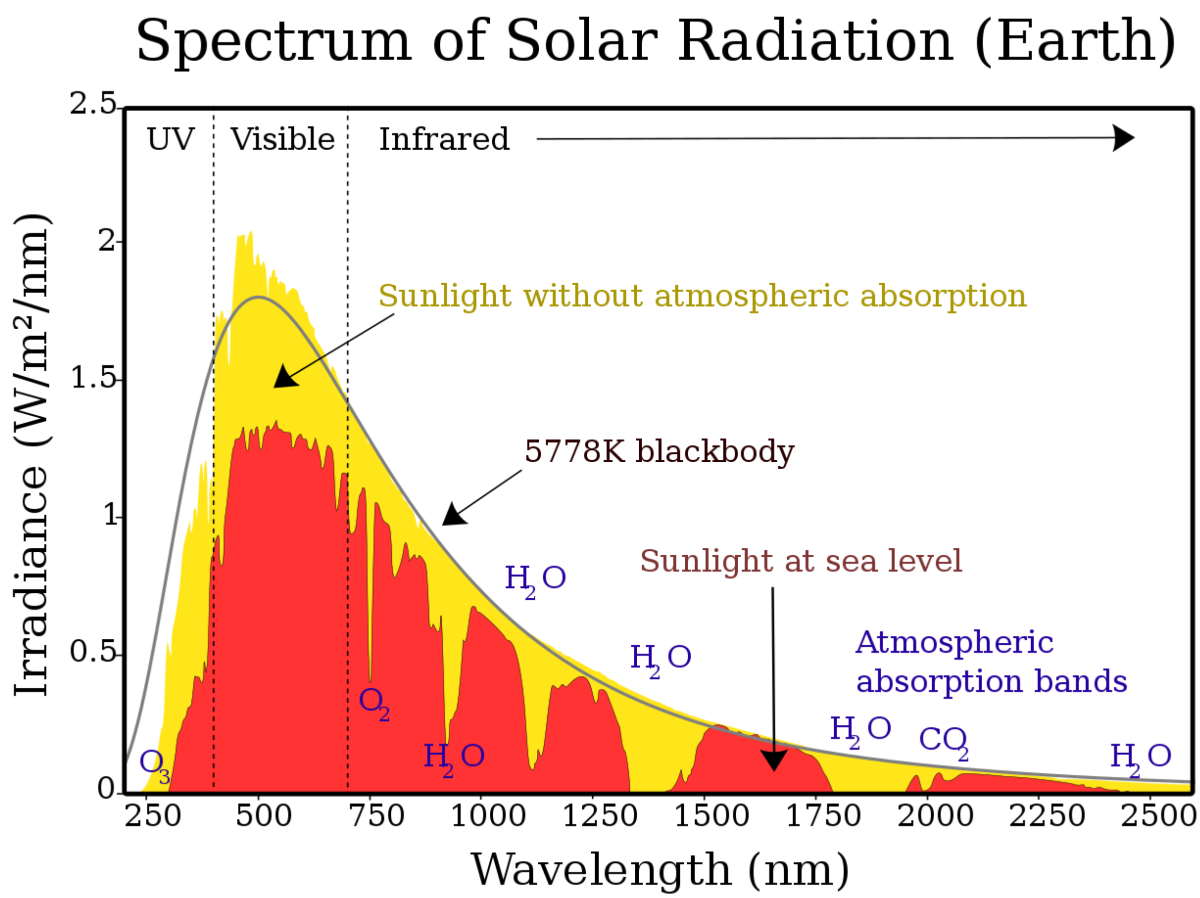


Figure 3.8: Spectrum of Solar Radiation (Irradiance Vs Wavelength) [52]

3.10.2 Parametric Sweep for Physical Values

Radius

Nanoparticles of each texture and model were simulated with varying radius starting from 20nm to 95nm (20nm, 40nm-80nm with 10nm steps, 95nm).

Height of nanoparticles

The position with respect to the bottom of the absorptive layer is denoted here as height, h_t in nm (Fig 3.10). The nanoparticles are placed at height, h_t =100 nm to 900 nm in 100 nm steps and simulated for every radius and wavelength.

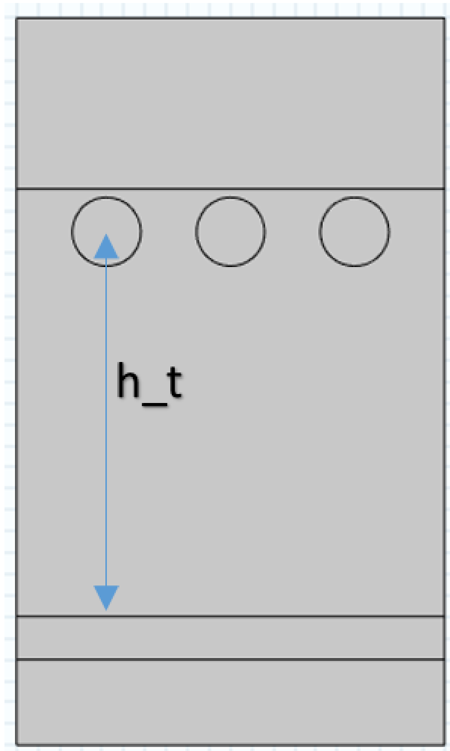


Figure 3.9: Parametric sweep for Physical values

3.11 Calculation of Absorption Efficiency

Using the S parameters (S11, S21) generated from our simulations we can calculated the percentage of power absorbed and from that the Spectral Absorption Rate (1).

$$P_{abs} = 1 - |S11|^2 - |S21|^2$$

$$SAR(\lambda) = \frac{\int P_{abs}(\lambda) I_{AM1.5}(\lambda) d\lambda}{\int I_{AM1.5}(\lambda)\, d\lambda}$$

This equation gives us a value which represents the average power absorbed as percentage over a range of wavelength. Here in this equation, P_{abs} represents power absorption, S11 represents the fraction of power reflected back to port 1 and S21 represents the fraction of power transmitted through port 2.

$I_{AM1.5}$ represents the standard irradiance of sunlight at earth's surface. It is defined at a specified orientation under a set of specified atmospheric conditions. It provides a standard reference for comparing the performance of different photovoltaic technologies.

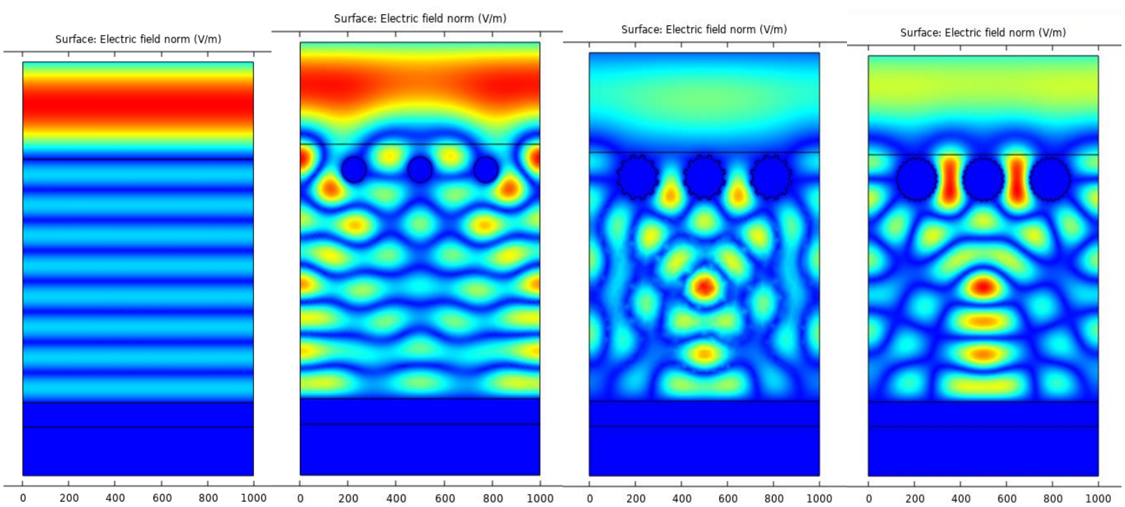
Chapter 4

Results

In our simulations, we have varied the textures of the nanoparticles used, their position within the absorptive layer and their radius. In this chapter, we present the results we have obtained from our simulations and the implications of these results.

4.1 Electric Field Pattern

We have tested out the response of the four different models of solar cells for light of wavelength from 400 nm to 1250 nm. The reason for choosing this range is that the intensity of sunlight reaching earth's surface is significant in this range. Figure 4.1 shows the electric field distribution within the solar cell when 900 nm wavelength light was applied to each of the models.



(a) (b) (c) (d)

Figure 4.1: The electric field response of (a) bare model; (b) Smooth nanoparticle model, (c) Texture 1 model; (d) Texture 2 model for light of wavelength 900 nm (nanoparticles placed at the topmost position)

In the electric field distributions, we see that compared to the bare model, there are large electric fields built up within the solar cells with nanoparticles. This enlarged electric fields are indicative of plasmonic effects around the nanoparticles. Thus, the application of nanoparticles within solar cells excite plasmonic effects within the solar cell which should in turn lead to greater absorption compared to the bare model.

4.2 Bare Model vs Smooth Nanoparticle

We compared the performance of the solar cells with and without smooth circular nanoparticles embedded within the absorptive layer. In the model with the nanoparticles, we varied the radii of the nanoparticles and also varied the height of the nanoparticles within the cell.

4.2.1 Absorption Spectra

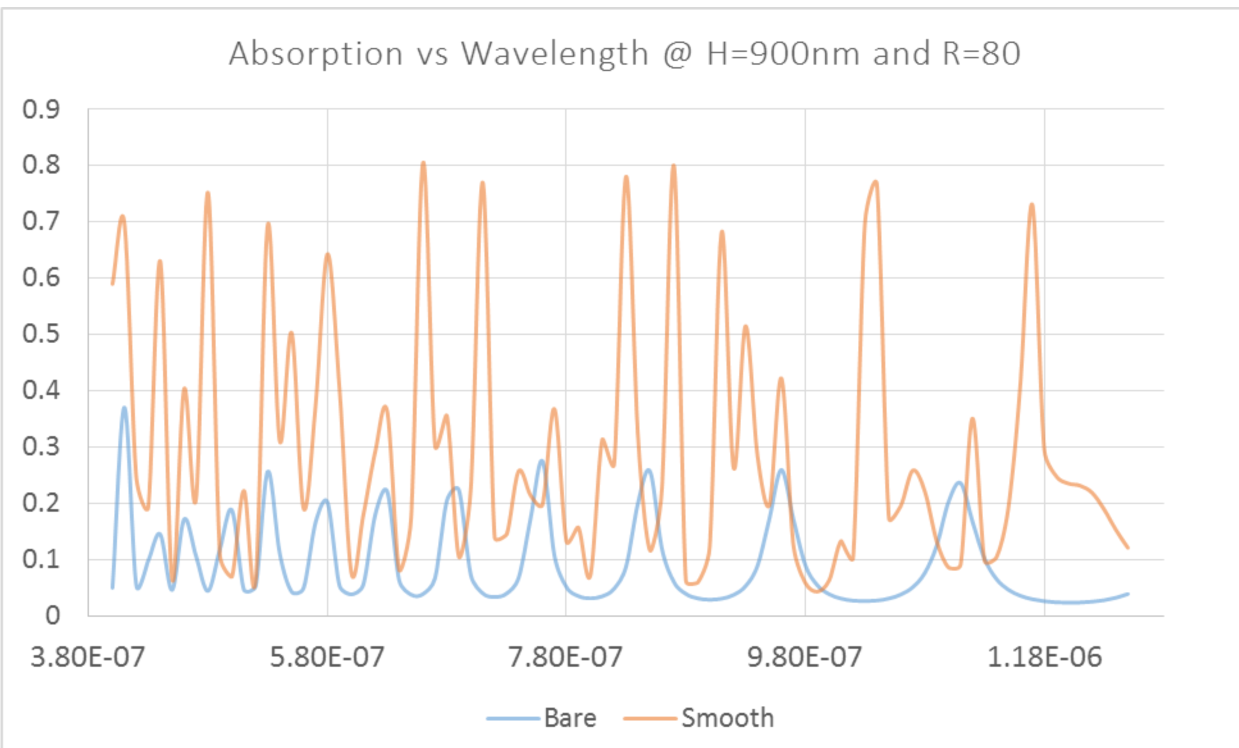


Figure 4.2 : Absorption vs wavelength plot for bare and smooth nanoparticle models

Figure 4.2 shows the absorption of light within the cell for both model. It's clear from a glance at the data that at almost all tested wavelengths the absorption of the nanoparticle models exceeds that of the bare model.

4.2.2 Optimal Radius and Position

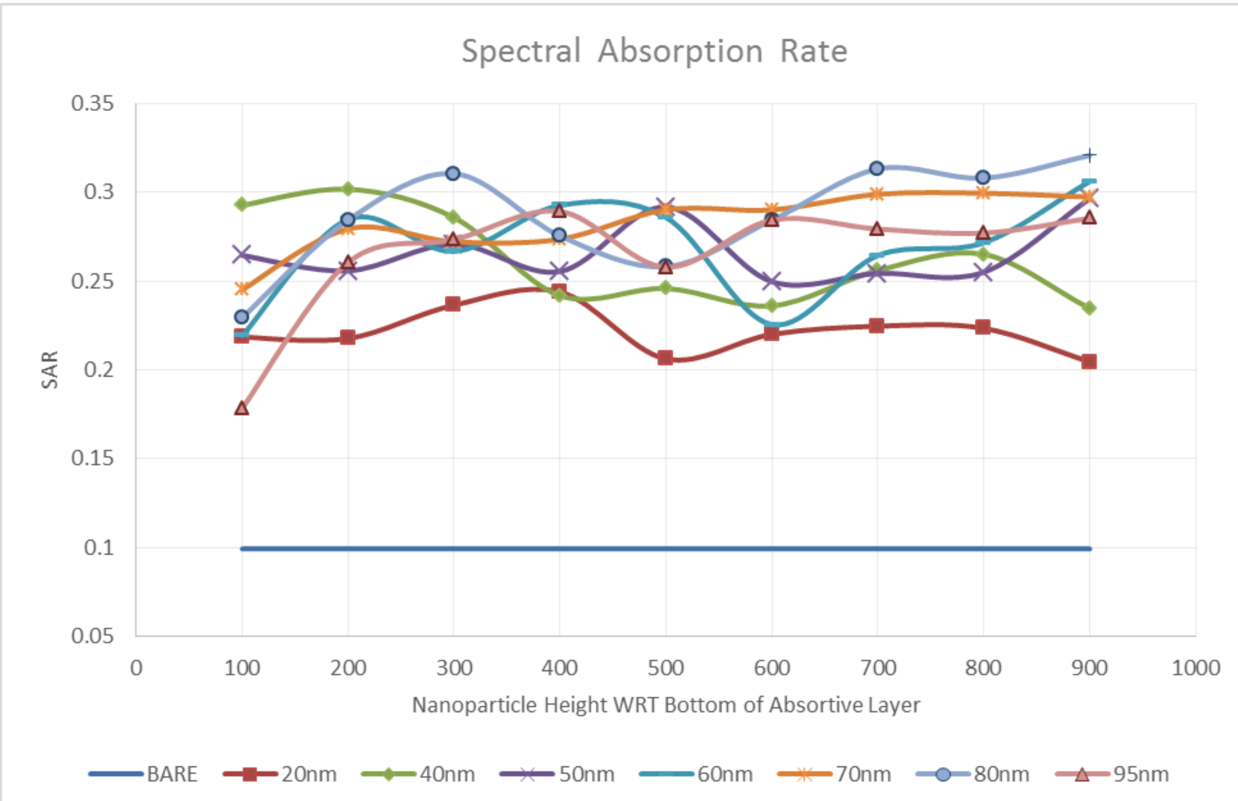


Figure 4.3 : SAR of Bare Model vs Smooth Nanoparticle Model with varying radius and position of nanoparticle

Figure 4.3 shows the Spectral Absorption Rate (SAR) of the models with nanoparticles varying in radius from 20 nm to 95 nm and also with varying height of the nanoparticles from the bottom of the cell to the top. With a close observation of the data presented in Figure 4.3 we see that the models with nanoparticles show significantly better SAR than the bare model irrespective of the position of the particles. But comparing between the models with the nanoparticles with different radii and position, we see a large variation of SAR. If we observe the peak of each of the curves, we'll observe that the best SAR for each radius is obtained when the particle is placed at a different position. Thus, this demonstrates that the optimal position of the nanoparticles varies with the radius of the particle.

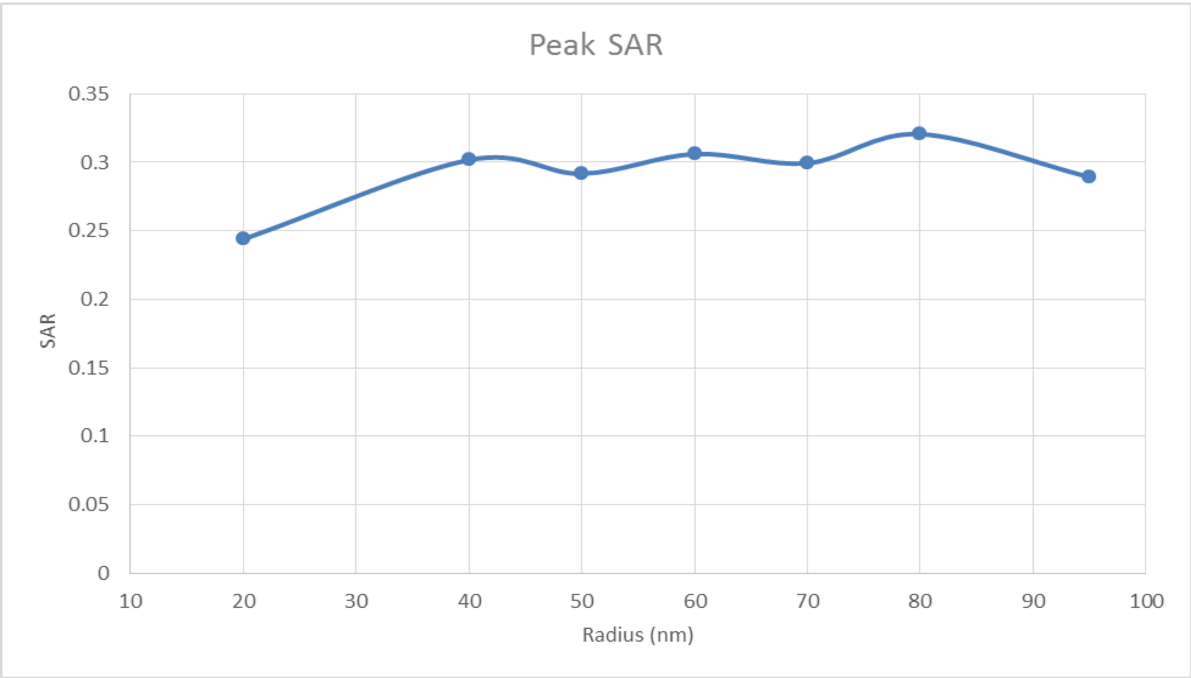
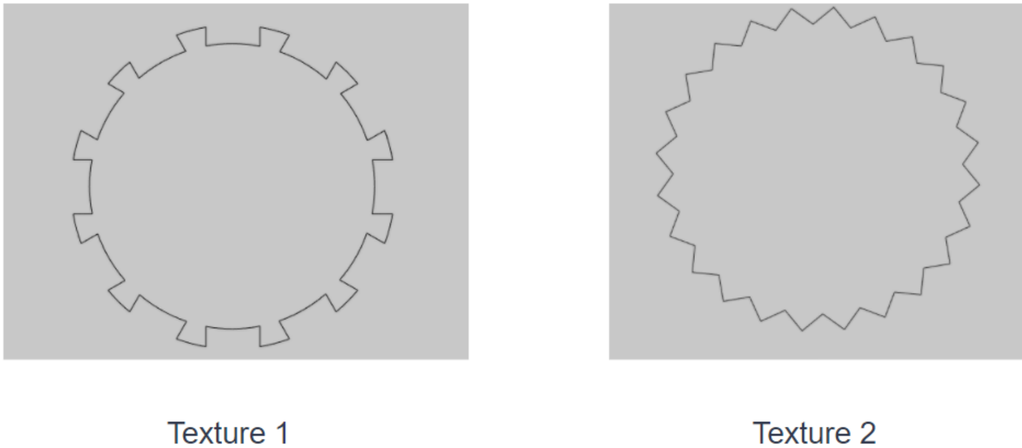


Figure 4.4 : Peak SAR obtained for nanoparticles of varying radius

Figure 4.4 shows the peak SAR obtained for different radii of nanoparticles. From this data, we see that the highest SAR was obtained for nanoparticles of 80 nm radius. This was obtained when the 80 nm particles were placed at the very top of the absorptive layer.

4.3 Smooth vs Textured Nanoparticles

From the previous section, it is clear that application of nanoparticles does improve the absorption within the solar cell. But, the question remains whether smooth smooth and circular nanoparticles are in fact the best choice of nanoparticles. To answer that question, we tested two different textured nanoparticles. Figure 4.5 displays the two different textures we used in our investigation.



a) b)

Figure 4.5 : a) Rectangular textured nanoparticle, b) Triangular textured nanoparticle

4.3.1 Choice of Size of Textured Nanoparticles

In the model with the smooth nanoparticles, we observed that the maximum SAR was obtained with nanoparticles of 80 nm placed at the very top of the absorptive layer. Because of this result, in our subsequent investigations with textured nanoparticles, we have used nanoparticles of 80 nm and have placed them at the top of the solar cell.

4.3.2 Comparison Between Textures

We have moved the textured nanoparticles within the absorptive layer to find out if applying the texture changes the optimal position of the particles. But, as we can see in Figure 4.6 for each of the textures, the optimal SAR was obtained when the particles were placed on top of the absorptive layer. This was likely due to the face that we chose 80 nm as the radius of the nanoparticles and thus the same result was obtained as in the case of smooth nanoparticles. But the point of real interest here is that, the maximum SAR obtained for each of the models were different. The triangular textured model gave the greatest SAR and the rectangular textured model being the second best. The smooth nanoparticle came out with the least SAR compared to the textured models. This shows that applying textured nanoparticles may provide a possible way of enhancing light trapping compared to that of regular nanoparticles.

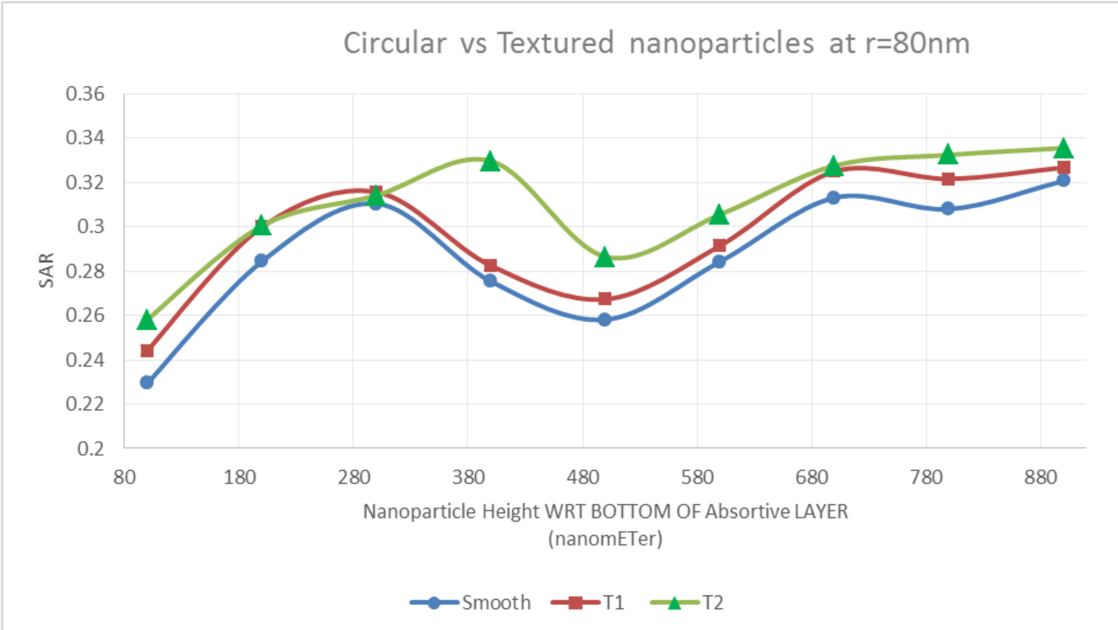


Figure 4.6: SAR of different textured models at varying heights

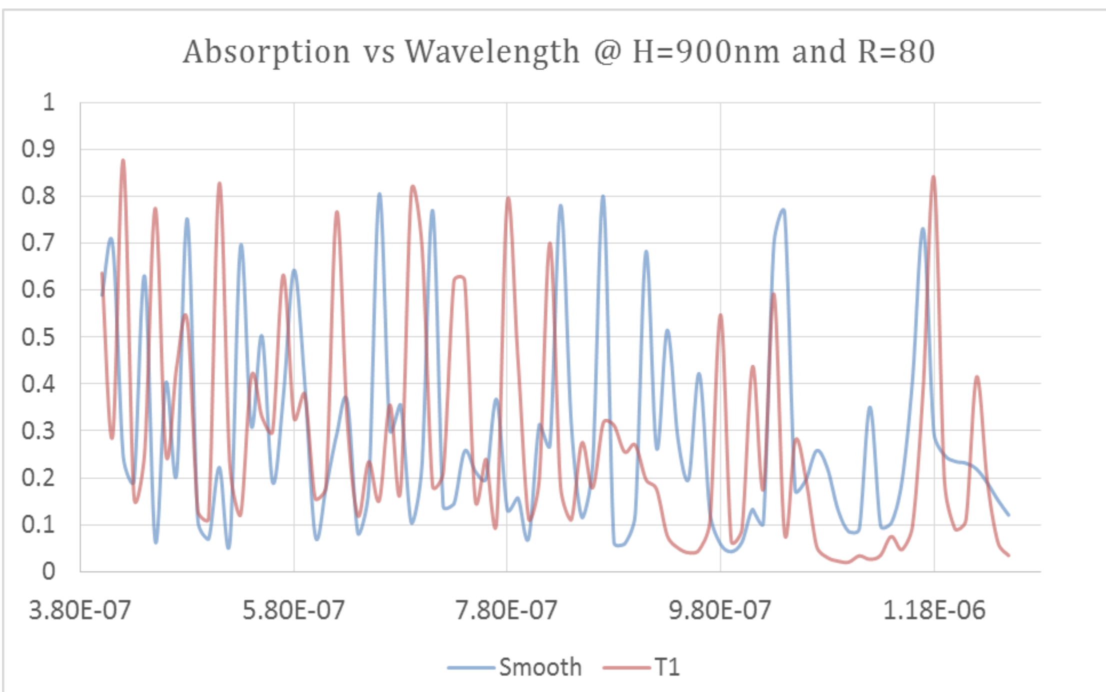


Figure 4.7 : Absorption vs wavelength of Smooth and rectangular textured model

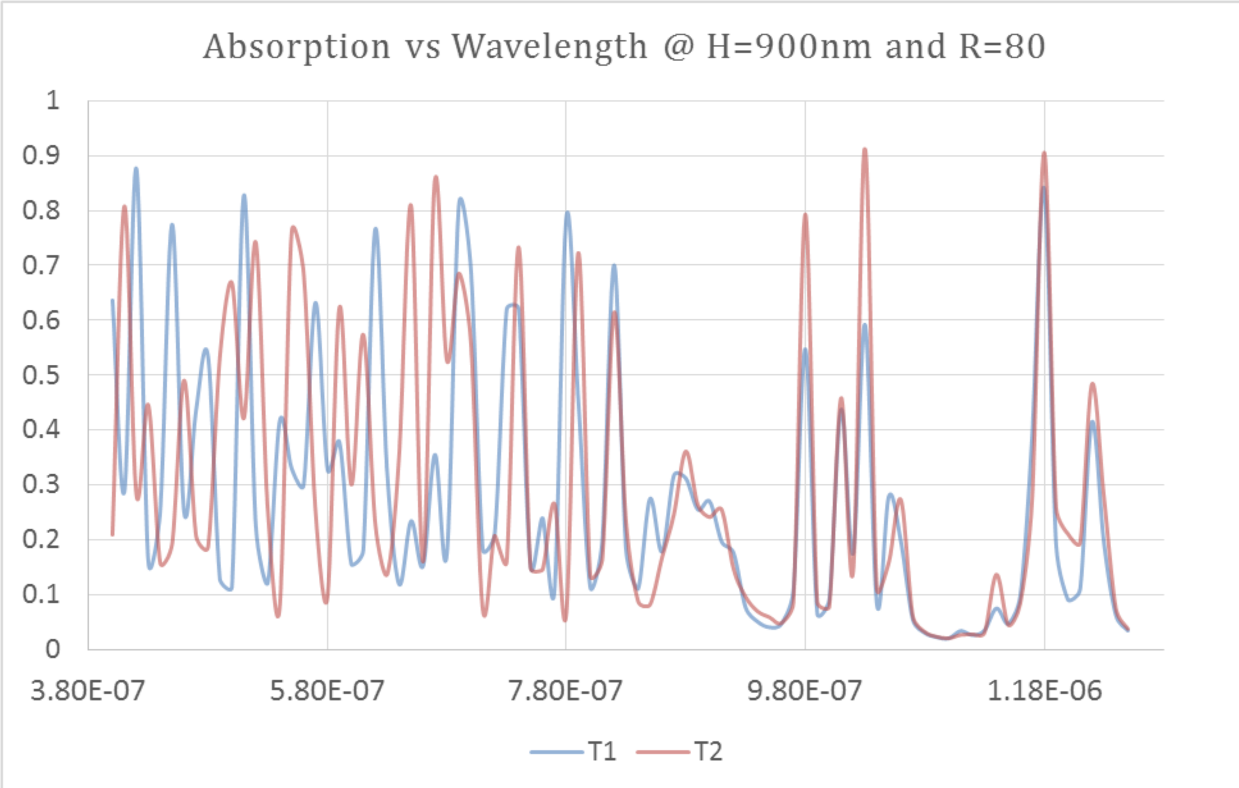


Figure 4.8 : Absorption vs wavelength of Rectangular and Triangular textured nanoparticle models

Figure 4.7 shows the absorption spectrum comparison between the smooth and rectangular textured model.

Figure 4.8 shows the same comparison between the two textured models. Unlike the case of the comparison between the bare model and the smooth nanoparticle model, the difference in performance between the different textures are relatively small and thus not clear from the absorption spectra comparison. But, the overall SAR of the different models were slightly different.

4.4 Multilayered Nanoparticle Model

In most of the literature, the focus has been on applying a single array of nanoparticles to the absorptive layer. Little investigation has been done to see the effect of applying multiple arrays of nanoparticles. To observe the effect of such an application of nanoparticles, we designed a model with 3 layers of circular smooth nanoparticle within the absorptive layer.

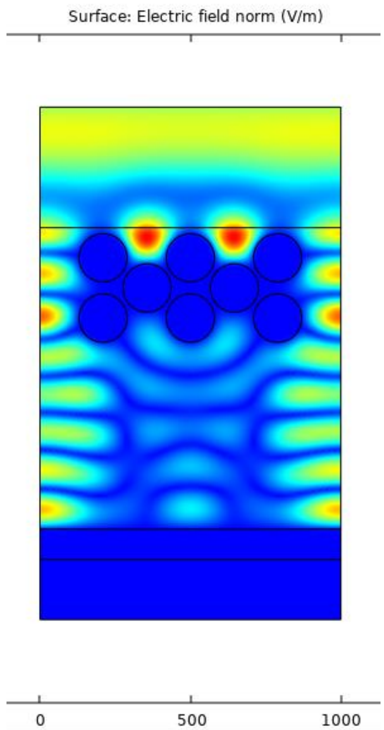


Figure 4.9 : Electric field response of multilayered nanoparticle model at 900 nm wavelength

Figure 4.9 shows, there is clearly large electric field built up within the absorptive layer due to the nanoparticles. This is indicative of SPR and possibly better absorption.

4.5 SAR Comparison of All Models

Table 4.1 shows a comparison of the best SAR obtained for all the different models we have tested out. It's clear that all the models with nanoparticles gave very large improvements compared to the bare model. This shows that the application of nanoparticles in solar cells is very much effective for improving the absorption of light within the cell. There was a trend of slightly better absorption for textured nanoparticles. Especially, the model with multiple layers of nanoparticles showed an outstanding improvement in absorption with SAR of 0.5780. Thus, it is apparent that application of multiple layers of nanoparticles could open up room for major improvements in light trapping.

Table 4.1 : SAR comparison between 5 different models

Model	Best SAR	% improvement compared to bare model
Bare	0.0993	0
Smooth Nanoparticles	0.3207	222.96
Rectangular Textured Nanoparticles	0.3267	229.00
Triangular Textured Nanoparticles	0.3355	237.86
Multilayered Nanoparticles	0.5780	482.07

4.6 Remarks

Our results show that the light absorption within TFSC can be enhanced significantly by the application of nanoparticles within the absorptive layer. The performance is further improved through the application of textures on the nanoparticles. An even greater improvement was observed when we applied multiple layers of nanoparticles. We also demonstrated that the optimal position of nanoparticles within a solar cell is dependent on the radius of the nanoparticles.

Chapter 5

Summary and Conclusion

5.1 Motivation for Our Work

The global energy demand has been increasing at a rapid rate for many years. But the main resource for our energy has been fossil fuel up to now. But eventually this resource will run dry. Thus it is crucial for us to prepare for the eminent energy crisis. To solve this problem, there has been a shift towards using more and more renewable sources of energy. Solar energy is among the primary renewable energy sources. Therefore, the research on solar cells have been very prolific in recent years.

Among the different types of solar cells, thin film solar cells (TFSC) primarily solves the problem of material cost and large scale production. It reduces the amount of material required to manufacture a solar cell. But, TFSC generally come with their own drawbacks of low efficiencies. To solve this problem, various light trapping mechanisms have been deployed. If the efficiencies of TFSC could be brought up to the level of wafer based solar cells, they would be revolutionary and would solve a major part of the energy demand related problems humanity is faced with in the 21^{st} century. Thus, we decided to conduct our work on improving the performance of TFSC.

5.2 Our Work

The use of nanoparticles within TFSC has been a promising area of investigation in recent years for the improvement of light trapping within TFSC. We have simulated multiple models including textured nanoparticles and multilayered nanoparticle array in TFSC with Al nanoparticles embedded within GaAs absorptive layer. All of the models have been compared with a bare model containing no nanoparticle.

Significant attention has been given to the use of Si as the semiconductor material for TFSC. But, some group III-V semiconductors such as GaAs have some distinct advantages over Si. They are-

- GaAs is a direct band gap material and therefore a more effective absorber.
- It has a more optimal band gap (1.42 eV) for terrestrial use.
- Higher absorption coefficient.

In spite of GaAs having these suitable characteristics, it has been largely unexplored. Thus, we opted to use GaAs as the absorbing semiconductor material to use for our investigation of light trapping.

As for the choice of material for the nanoparticles, Singh and Verma [40] demonstrated that using Al nanoparticles leads to more absorption of light in the semiconductor and less absorption in the nanoparticle itself, compared to other common metals such as Ag, Au and Cu. Therefore we chose Al nanoparticles to conduct our work.

Significant improvement in the spectral absorption rate was observed in all the models compared to the bare model. Particularly, the application of multilayered nanoparticles showed the greatest enhancement of absorption within the TFSC. Thus, we present the application of textured and multilayered nanoparticle arrays within the solar cell as a viable method for improving the optical path length of light within the cell and effectively improving the light absorption within the cell.

5.3 Future Works

Our work, in conjunction with other similar works shows that application of Al nanoparticles in GaAs absorptive layer is an effective method for increasing the absorption of the TFSC which in turn leads to greater efficiency of the device considering constant internal quantum efficiency. The use of multiple layers of nanoparticle arrays within the cell represents a scope of further investigation in the future. As the textured nanoparticles showed improved performance compared to the smooth nanoparticles, a possible area of exploration may be models where multiple layers of textured nanoparticles are used. A combination of our suggested method with preexisting methods may also be explored. A limitation of our work is that we did not take into consideration the periodicity of the nanoparticle arrays. An immediate extension of our work can be to manipulate the periodicity of the nanoparticles to optimize this parameter and thus further improve on the optimal conditions we obtained. For our work, we chose GaAs as the group III-V material. But there are other promising materials that provide similar advantages as GaAs. A repetition of the works mentioned here in other group III-V materials could lead to good results. To follow up our work in this thesis, we plan to include these modes of investigation.

5.4 Conclusion

In this thesis, we have illustrated our work on “Light Trapping Optimization in GaAs TFSC using Al Nanoparticles”. Our main goal was to observe the effect on light absorption when Al nanoparticles are applied in various ways in GaAs solar cells and to find an optimum configuration of the nanoparticles. Several lines of research has indicated that GaAs is a viable option for being used for the absorptive layer. Thus we chose it as the semiconductor for our absorptive layer. In our work, we modeled several different types of application of nanoparticles in GaAs TFSC and showed that through optimizing the configuration of the nanoparticles, large enhancements in absorption can be achieved. Multiple layers of nanoparticles applied to the absorptive layer showed the most promise. Comsol Multiphysics software was used to carry out these investigations.

Our work adds to the growing body literature that looks into the effect of applying nanoparticles in TFSC. Most of the relevant work including ours show significant enhancement of performance of TFSC through the use of nanoparticles. With the promise this approach has shown, in the near future, a large chunk of your energy demands might just be met through the merger of photovoltaic and nanoparticle technologies. We conclude our thesis with the hope that photovoltaic technology very soon provides the very much needed solution to the eminent energy crisis of the world.

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