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Présentée par : **Mokrane Mohamed**

Thème

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Light Trapping in Solar cells Based on Silicon

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Light trapping in solar cells based on silicon

Abstract

Mohamed Mokrane

The main purpose of this project is to understand the domain of photovoltaic and to master how to increase light absorption in solar cells, based on silicon as an active layer, to enhance their efficiency by light trapping using some theoretical work. One of the most important techniques and ways used to enhance light absorption is changing the surface state by texturing or refractive gratings to get a total reflexion of light. In this project we focused on the second part (surface refractive gratings) and our principal idea is to imagine a surface with different geometries based on different periods of gratings. We dealt also with effective medium and surface reflexion points to understand the evanescent field. The findings of this research strongly indicated that the period of gratings plays a crucial role in the grating equation and the refractive index of the effective medium is very important.

Keywords

Light trapping, solar cells, Semi-conductors, Defects, Silicon.

Piégeage de la lumière dans les cellules solaires à base de silicium

Résumé

Mohamed Mokrane

L'objectif principal de ce projet est de comprendre le domaine du photovoltaïque et de maîtriser comment augmenter l'absorption de la lumière dans les cellules solaires, à base de silicium comme couche active, pour améliorer leur efficacité par piégeage de la lumière à l'aide de travaux théoriques. L'une des techniques et des moyens les plus importants utilisés pour améliorer l'absorption de la lumière consiste à modifier l'état de surface par texturation ou réseaux de réfraction pour obtenir une réflexion totale de la lumière. Dans ce projet, nous nous sommes concentrés sur la deuxième partie (réseaux de réfraction de surface) et notre idée principale est d'imaginer une surface avec différentes géométries en fonction de différentes périodes de réseaux. Nous avons également traité les points de réflexion totale au niveau de surface pour comprendre le champ évanescent. Les résultats de cette recherche ont fortement indiqué que la période des réseaux joue un rôle crucial dans l'équation du réseau et que l'indice de réfraction du milieu effectif est très important.

Mots clés

Piégeage de la lumière, Cellules solaires, Semi-conducteurs, Défauts, Silicium.

محاصرة الضوء في الخلايا الشمسية القائمة على السيليكون

ملخص

محمد مقران

الهدف الرئيسي من هذا المشروع هو فهم مجال الخلايا الكهروضوئية وإتقان كيفية زيادة امتصاص الضوء في الخلايا الشمسية ، استنادًا إلى السيليكون كطبقة نشطة ، لتحسين كفاءتها عن طريق محاصرة الضوء بمساعدة العمل النظري. من أهم التقنيات والوسائل المستخدمة لتحسين امتصاص الضوء تغيير تشطيب السطح عن طريق التركيب أو صريف الانكسار لتحقيق الانعكاس الكلي للضوء. ركزنا في هذا المشروع على الجزء الثاني (حواجز الانكسار السطحي) وفكرتنا الرئيسية هي تخيل سطح به أشكال هندسية مختلفة وفقًا لفترات مختلفة من حواجز شبكية. لقد عالجنا أيضًا نقاط الانعكاس الإجمالية على مستوى السطح لفهم المجال الزائل. أشارت نتائج هذا البحث بقوة إلى أن فترة الشبكة تلعب دورًا مهمًا في معادلة الشبكة وأن معامل الانكسار للوسط الفعال مهم جدًا.

الكلمات الدالة

محاصرة الضوء ، الخلايا الشمسية ، أشباه الموصلات ، العيوب ، السيليكون

Citation

Soit A un succès dans la vie. Alors A = x + y + z, où x = travailler, y = s'amuser, z = se taire.

"Let A be a success in life. Then A = x + y + z, where x = to work, y = to have fun, z = to be silent."

"Lass A ein Erfolg im Leben sein. Dann ist A = x + y + z, wobei x = arbeiten, y = Spaß haben, z = schweigen."

لنكن" أ "ناجحًا في الحياة. ثم أ = س + ص + ض ، حيث س = للعمل ، ص = للاستمتاع ، ض = أن تكون "
" صامتًا

Albert Einstein
Mathématicien, Physicien, Scientifique (1879 - 1955)

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General Introduction

General introduction

In nature, we have four states of mater; solid, liquid, gas and plasma, and a lot of combinations of interfaces between these states are possible like the solid–liquid, the solid–gas, and the liquid–gas interfaces. The term surface is often used synonymously, although interface is preferred for the boundary between two condensed phases and in cases where the two phases are named explicitly. Interfaces can also separate two immiscible liquids such as water and oil [1].

The world is facing a lot of problems; like pollution plus climate changing and the fossils with nuclear fuels energies are not safety and cannot satisfy the humanity in next years due the increasing of consummation and need. For these reasons renewable energies especially solar cells can be a good solution of the societies. The structure of the cell is based on the contact between different mono-layers of materials like silicon (Si), under its different structures, and oxides semi-conductors [2]. The position of Algeria, in the globe, is very important and our country can play a crucial role in the market of solar energy if we know and master how to take benefit from the sun we have.

The most important layer in the solar cell is the active one which can be made from a material that can absorb sun light, to produce electron-hole pairs, like silicon, oldest and well studied semi-conductor with a gap of 1,12 eV at room temperature. The (Si) can be found under different structures crystalline, amorphous (a-Si), hydrogenated amorphous (a-Si:H) and microcrystalline silicon (μ-Si:H) [3].

The big problem of the solar cell with a simple geometry is the weak efficiency and the photo-degradation with time. When shining the cell, light rays enter it through the front surface and if not absorbed, leave through the rear surface of the cell. Extending the path of light inside the cell, referred as optical confinement or light trapping, is a sophisticated way to increase the probability of absorption and reduce the thickness of the layer [4]. Light trapping is one of the major topics in solar cell research today and concerns every type of solar cell. One way to realize this objective is to increase the internal path length of light inside a solar cell by diffraction with optical nanostructures. The main idea behind this is that the structure changes the direction of the incident light to make it traveling as long as possible in the solar cell. Surface texturing and diffractive gratings are one type of optical nanostructure that

reveals great potential in this domain. Diffractive gratings for c-Si solar cells were investigated by Heine and Morf in 1995. Solar cells become more important and at the same time thinner and thinner; thus research interest on diffractive gratings has renewed, and gratings have been investigated for all kinds of solar cell materials, including a-Si:H and organic compounds [5].

The aim purpose of this project is to understand and master the light trapping inside the solar cell based on silicon as active layer. In addition to this general introduction, the manuscript is divided into two main chapters:

> Chapter I concerns with general ideas and concepts of matter from the microscopic state till the macroscopic one. We indicate the silicon and P-N junction plus the structure of solar cell and current generated by absorbed light.

> Chapter II deals with the theoretical part concerning light trapping by diffractive gratings. In this part, we will deal more precisely with the grating equation where the parameter of period is very important to enhance light. We proposed different geometries to see how changing slightly the period can affect light trapping. Another important idea is the effective medium and its theory because the refractive index of the mixture of different materials plays an important role too. We finished this chapter by talking about the evanescent field at the point of the total reflexion.

We will conclude this manuscript by a general conclusion in which we summarize the main results and efforts of the present study.

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Chapter 1

Light and Matter: Solar cell

1.1. Introduction

The Greeks had distinguished four elements of nature: air, water, fire and earth, and with time science has become more mature to pick up two elements from those four elements which are light and matter. Since light and matter are in the same universe, they have to interact with each other. These interactions have been widely studied in the two past centuries. One of the main studies was the photoelectric effect by the German physicist and the father of modern physics A. Einstein, who said that the interaction between light and some kinds of materials induces photoelectric current [1]. In this chapter we are going to discuss these interactions in detail and talk about those materials in particular.

1.2. Light matter interactions

The domain of the light-matter interaction involves a wide range of physical phenomena such as classical and quantum electrodynamics, black holes and neutron stars, mesoscopic plasmonics, nanophotonics and subatomic quantum objects. The term interaction means that light and matter are two different things that influence each other somehow. The famous equation of Einstein $E = mc^2$ indicates that light and matter are two sides of the same coin correlated by the speed of light squared. Since light and matter are the components of the universe, their interaction is meaningful and worth studying. The history of scientific research from the earliest times to the present day can be summed up precisely in three questions: What is the nature of light itself ?, what is the nature of matter itself ?, and what is the nature of the reactive factor? [2].

1.2.1. Nature of matter

Matter is the "stuff" of the universe: air, water, planets, students, anything that has mass and volume, and it has four main physical states: Solid, liquid, gaseous, plasma. But what we care about is the small parts that make up matter and gives its microscopic and macroscopic properties [3].

1.2.1.1. Atom

Zooming a piece of material millions of times using a very advanced microscope (which is far to be built) may allow us to see the elementary unit of matter which we call the atom (atomos in Greek, which means "uncuttable"). The history of atom has seen different models starting from English chemist John Dalton model In the early 1800s [4] passing from the

Joseph John Thomson, Ernest Rutherfor [5] and Niels Bohr model which was in 1913 [6, 7] till the quantum mechanical model [5] named after the physicist Erwin Schrödinger who say that the atom constitutes from the positively charged nucleus centred at the middle surrounded by the negatively charged eletron's cloud [8].
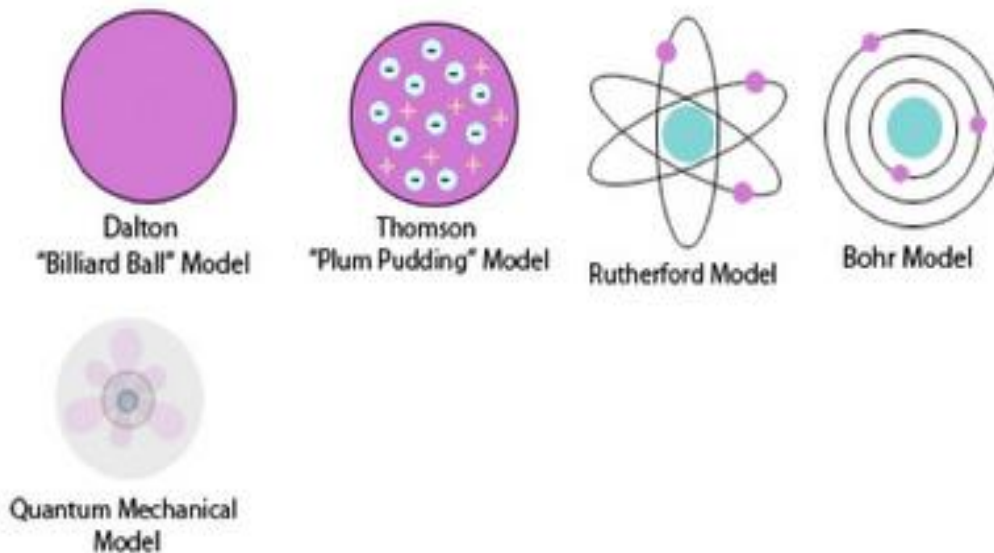

Fig.1.01. The atom models [9].

There are 92 different kinds of atoms that occur naturally in the world. Also, more than 20 heavier atoms have been produced artificially in the laboratory, and every molecule that makes up matter is made up of a specific group of atoms [10].

1.2.2. The nature of light

Allah (God) created our eyes in which we can only see a tiny fraction of the light spectrum. All the light, in other words, all electromagnetic waves [11] that we can detect during the day, is coming strictly from the sun which includes a lot of different spectra according to its wavelength.

In the early 1800s, scientists described light as a wave that is characterized by a wavelength or/and frequency depending on the interference effects in light beams that were shown at the experiments that were done by Thomas Young, François Arago and Augustin Jean Fresnel. Until the 1860s, the light was considered as part of the electromagnetic spectrum. However, by the late 1800, the scientists had faced a problem by the time they were dealing with the spectrum of the heated objects that could not be explained using the wave-based equations of light [12]. Two german physicists Max Planck and Albert Einstein solved

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this controversy. In 1900 the term quanta of energy was proposed by Planck which means that light is indiscernible bundles of energy [13]. By 1921 Einstein had confirmed the idea of the quanta of light when he was examining the photoelectric effect (the release of electrons from certain metals and semiconductors when struck by light) [14]. Thus the two physicists, Planck and Einstein, became Nobel laureates in 1918 and 1921, respectively and they called the quanta of energy of light the name "photon" [12].

After Planck and Einstein's explanation, quantum mechanics describes light both as particle and wave [15]. For photovoltaic applications, quantum mechanical description of light is rarely used, thus we are going to focus on the wave nature of light in particular.

As a classical wave, the wave nature of light is also characterized by frequency, wavelength and energy. The energy and the frequency are related by the Planck-Einstein equation [16].

$$E = h\upsilon \qquad (1.01)$$

E : The photon energy

h : Planck's constant

υ : The frequency of the wave

Where the wavelength and the frequency are related by the given equation:

$$\upsilon = \frac{c}{\lambda} \qquad (1.02)$$

C : The speed of light
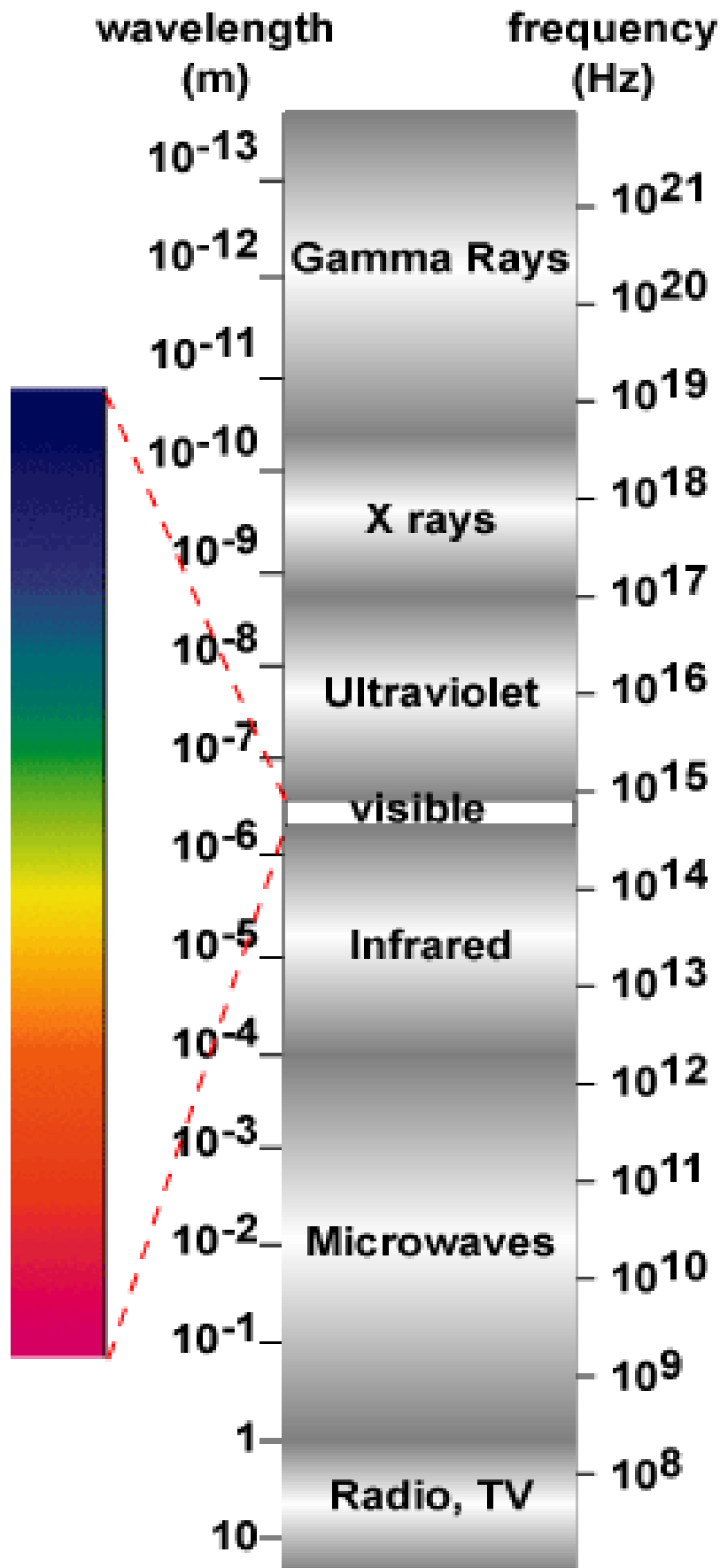
λ : The wavelength of the light

Fig.1.02. The electromagnetic spectrum [12].

1.2.3. Light and matter interaction

When light interacts with an atom several things may happen such as absorption transition and reflection and after the interaction the atom might gives back some light or photons.

➤ **Absorption and emission**

In fact, electrons move around the nucleus to some extent similar to the planets orbiting the sun. The electrons are not localized at some position but they form a cloud of probability where one of them is likely taking an orbit with a particular probability. Each of those orbitals has its specific energy. If we have an atom with two different orbitals with energies and where the difference between them is;

$$\Delta E = E_2 - E_1 \qquad (1.05)$$

At the first the electron is taking the orbital with the lowest energy, E_1, if a photon with an energy ΔE interacts with the atom, then the electron absorbs energy and goes to the orbital with the highest energy E_2 [17].

Fig.1.03. (a) Absorption and (b) emission processes [17].
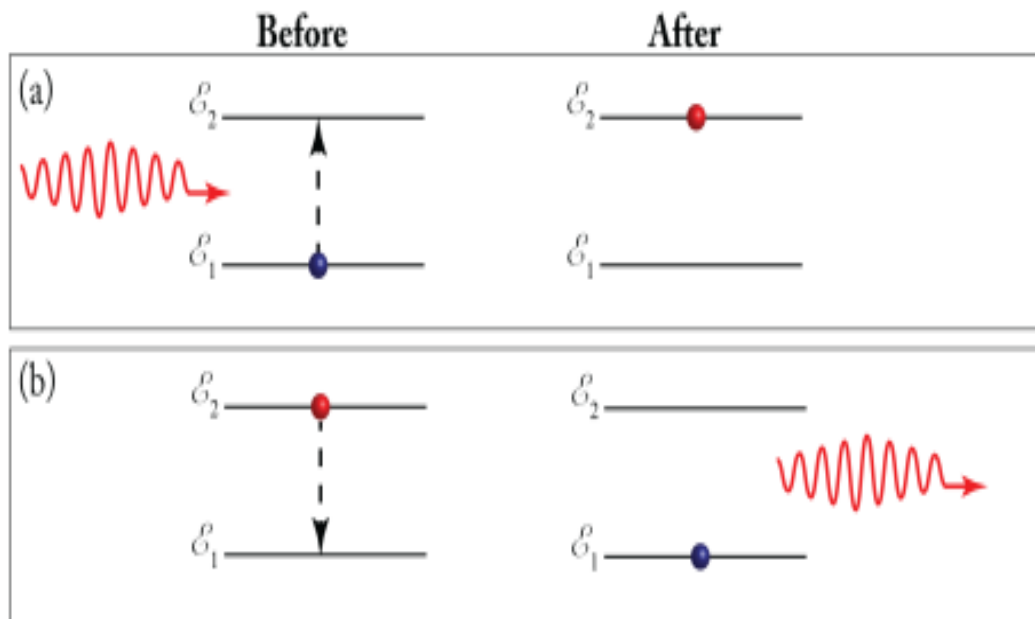
After a while the electron tends to lose the extra energy in form of a photon with the energy ΔE, and goes back to the first orbital that is the process of emission.

1.3. Solid state

Solid-state has been divided into three major sectors according to their electronic structure (the band gap energy) which are metals, insulators and semiconductors which are very

important and useful in the photovoltaic domain. Thus, we should concentrate on them to understand well their properties.
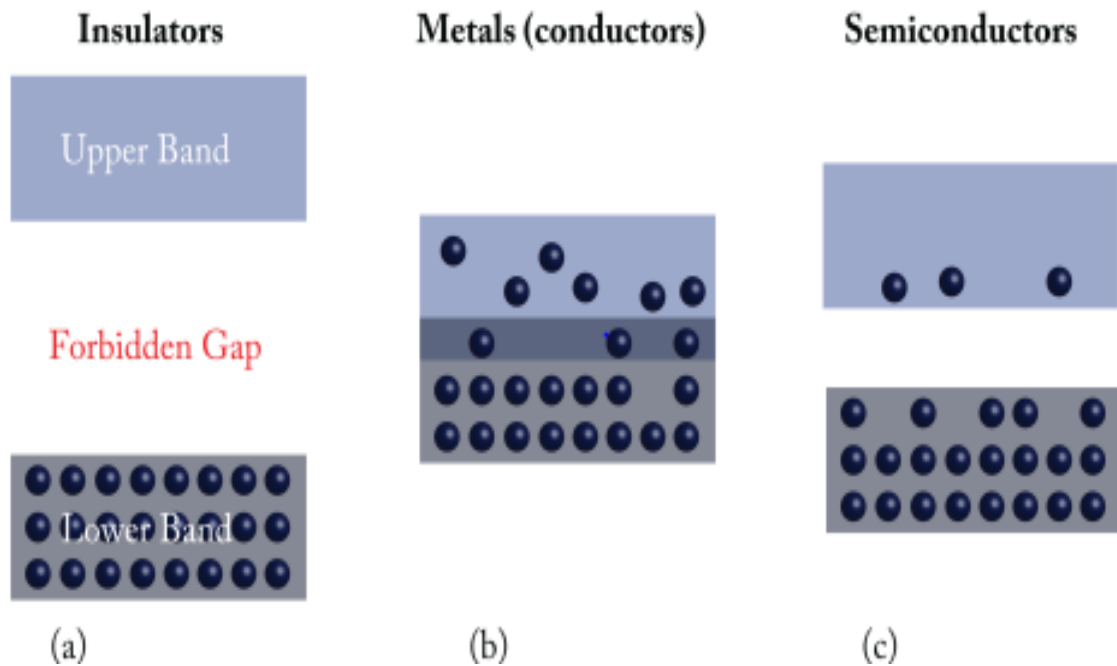

Fig.1.04. Schematic representation of (a) insulators, (b) metals (conductors), and (c) semiconductors with their corresponding energy bands and band gaps [17].

1.3.1. Semiconductors

The history of semiconductors starts all way back to 1874, with the work of Braun who discovered the asymmetric nature of electrical conduction between metal contacts and semiconductors, such as copper, iron, and lead sulfide [18]. Semiconductors (SCs) are usually classified between the metal and the insulators depending on their resistivity (or the conductivity), where the last is ranging between $10^{-2}\,\Omega$ to $10^{10}\,\Omega$ in the case of the SCs. In other words, we can also classify the materials in terms of their band gap energy as indicated in Fig.1.04 where semiconductors have band gap energy between zero and 4 eV. For example, the most common semiconductor in the world is the silicon (Si) and Germanium (Ge) with band gap energy equals to 1.12 eV and 0,67 eV, respectively, at room temperature. Besides the Si, there are a lot more semiconductors found in nature such as zinc-blende (ZnS) cuprite (Cu2O), and galena (PbS) [19].

We can localize the pure semiconductors in the IV group. where the compound semiconductor materials, most of which are formed from special combinations of group III with group V and group II with group VI elements on the periodic table as indicated in fig. 1.05 [17].
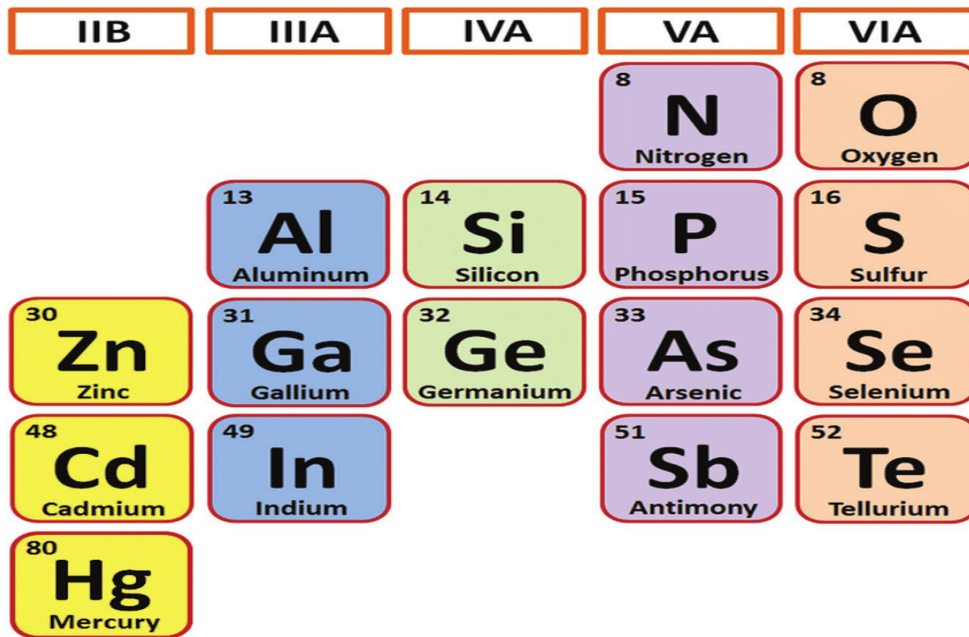
Fig.1.05. The elements in the periodic table to form possible semiconductor solid [12].

Pure semiconductors, like Si and Ge, crystallized in the diamond structure, while other semiconductors are mostly stable in the zinc blend structure which is similar to the diamond one as illustrated in figure.1.06 [19]
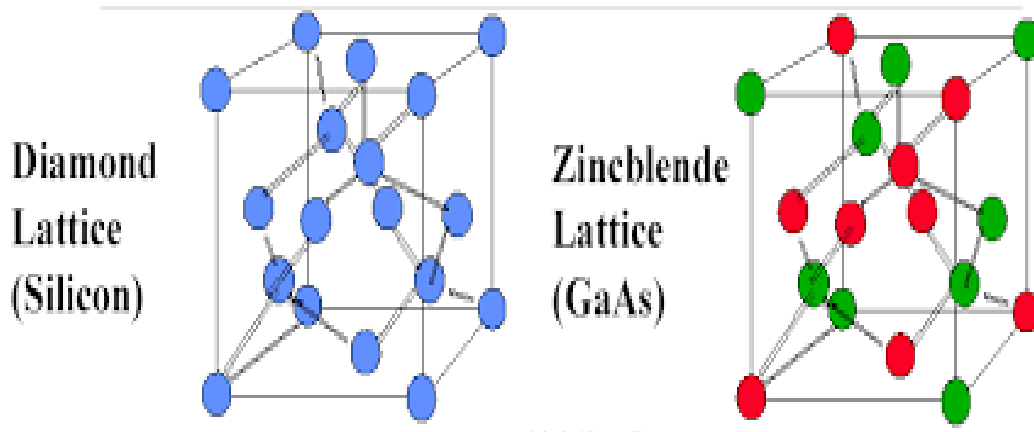
Fig.1.06. The crystal struture of silicon and gallium-arsenide [20].

1.3.1.1. Monocrystalline silicon

Monocrystalline silicon is a crystal where its atoms are arranged according to the diamond structure with an interatomic distance d = 2.37 Å. The bonds between atoms are type 3sp3 and the corresponding energy bands are the valence and conduction ones separated by a band gap of about 1.12 eV.

The width of the E_g gap determines the exchange of charge carriers between the different energy bands and thus the electronic properties of the semiconductor [21].
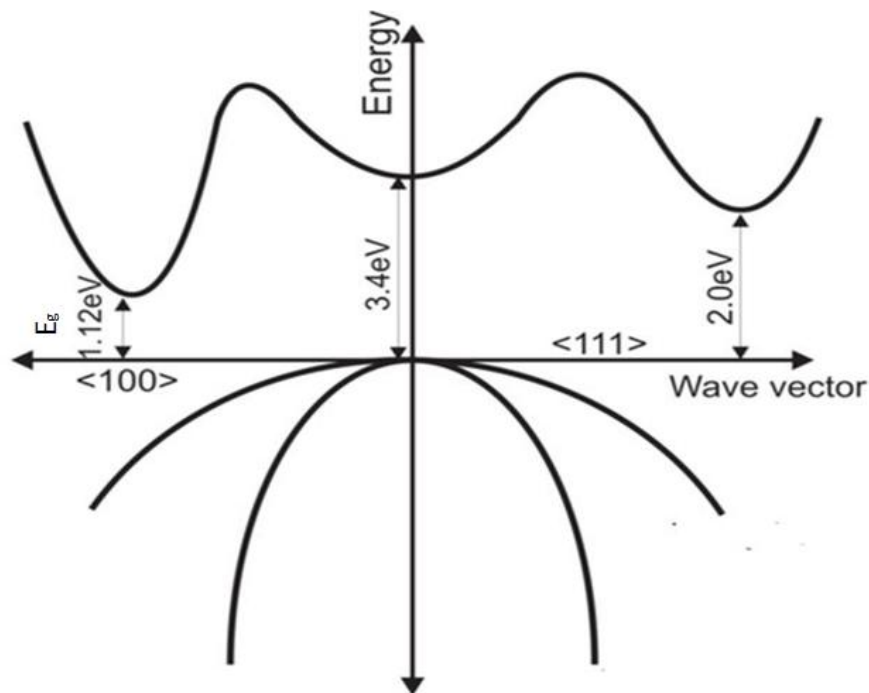
Fig.1.07. Band structure of silicon [22].

Plus the crystalline structure, the silicon can exist in an opposite structure which is the amorphous one where a lot of distortions exist and we lose the order in long distance

1.3.1.2. Amorphous silicon (a-Si)

Figure (1.08) shows the disorder existing in the amorphous structure and Figure (1.09) shows the energy bands of crystalline and amorphous silicon. The distortions which appear in amorphous silicon introduce localized states in the forbidden band. These distortions can give rise to the formation of dangling bonds. These bonds, which can be neutral, positively or negatively charged, influence the electronic properties of amorphous silicon. Dangling bonds (D) or unsatisfied bonds are therefore very efficient electron traps. The single electron can also eventually leave the atom, leaving a positively charged center [23].

Amorphous silicon has advantages over crystalline silicon such as:

- Possibility of depositing it on large surfaces;
- Possibility of depositing it on large and flexible surfaces
- Easy of manufacture;
- Strong absorption of visible light;
- Little degradation by x-rays;

- Higher band gap (1.75 eV; 1.12 eV for crystalline silicon), which allows amorphous silicon also has some drawbacks:
- Lots of flaws in the structure;
- Low mobility of free carriers;

This comparison does not mean that amorphous silicon can replace crystalline silicon, but it is useful in areas where crystalline silicon cannot be used. Among the applications of amorphous silicon we can indicate (mention):

- Telefax applications
- Xerography applications
- Flat screens

(a)   (b)
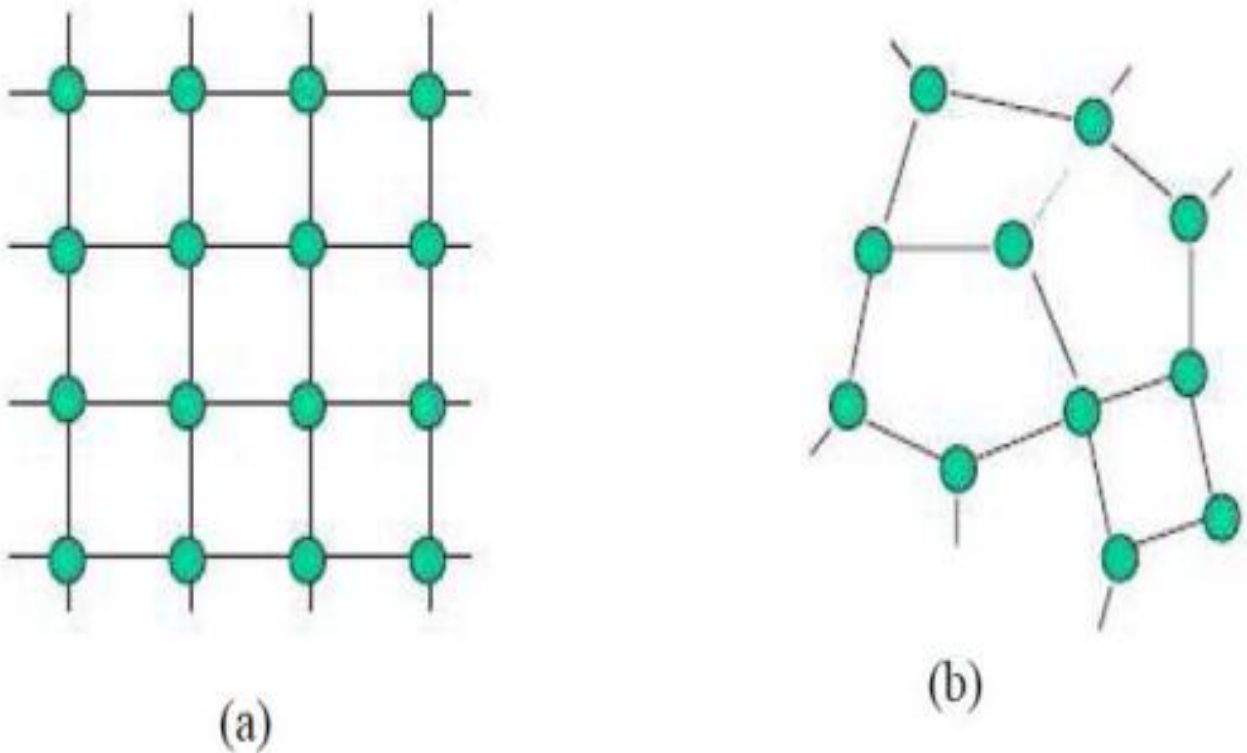
Fig.1.08. Schematic view of the atomic arrangement in the structure: (a) crystalline, (b) amorphous [30].
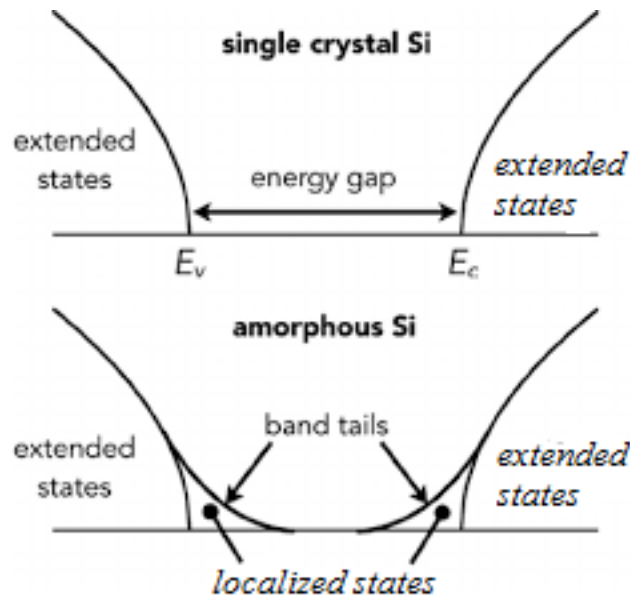
Fig.1.09. Density of states in crystal structure, and amorphous structure of Si [31].

➢ **Current**

We know from the previous sections that light can be absorbed by the electrons. The same case happens here with the semiconductors, where their valence electrons absorb light, the energy of light must be equal or greater than the band gap energy of the semiconductors, and go to the conduction band leaving behind holes in the valence band (the absence of an electron) resulting in a flow of current running in the semiconductor [12]**.**
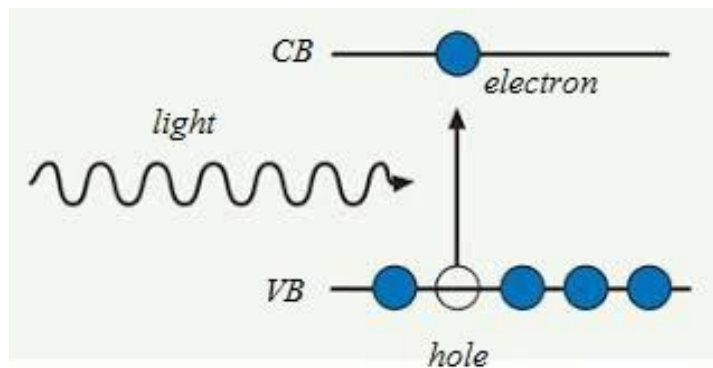
Fig.1.10.The creation of electron-hole pairs.

➢ **Doping**

Doping is one of the important processes in semiconductor physics which is used to manipulate the number of charge carriers in the valence and the conduction band of the semiconductors. When we dope the elements of the IV group from the periodic table by the elements of the V, we get N-type semiconductor, in which the majority carriers are the electrons. On the other hand, P-type semiconductor is the one in which the majority of carriers

are the holes. P-type semiconductors obtained by doping group IV elements using the elements of group III [23].
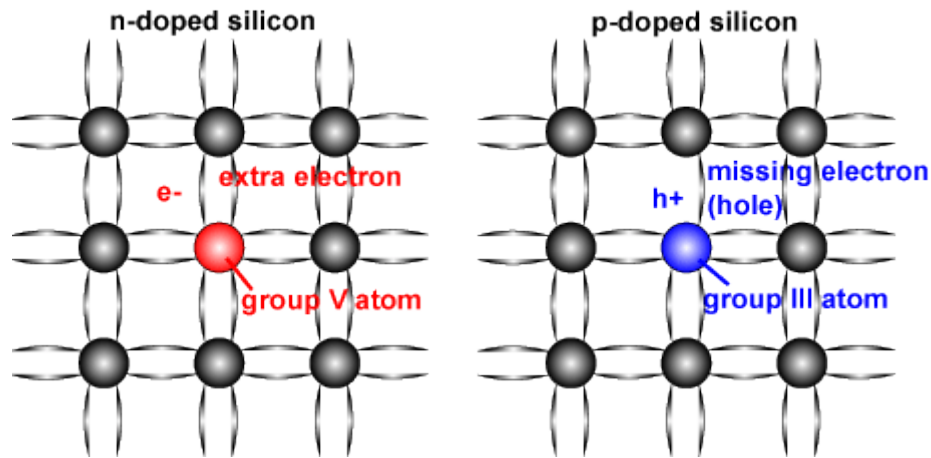
Fig.1.11. Schematic of a silicon crystal lattice doped with impurities to produce n-type and p-type semiconductor material [12].

1.4. P-N Junction

New physics always comes from putting different stuff together. We saw in the previous section that we have n and p type of semiconductors, thus, what happens if we bring those two types together?

Bonding of the n-type material with the p-type material (figure 1.12) causes the excess electrons in the n-type material to diffuse to the p-type side and the excess holes of the p-type material to propagate to the n-type side. On the other hand, The movement of electrons to the p-type side exposes the positive ion nuclei to the n-type side while the movement of the holes to the n-type side exposes the negative ion nuclei to the p-type side, resulting in an electron field at the junction and forming the depletion region. Furthermore, the voltage results from the electric field formed at the junction [24, 25].
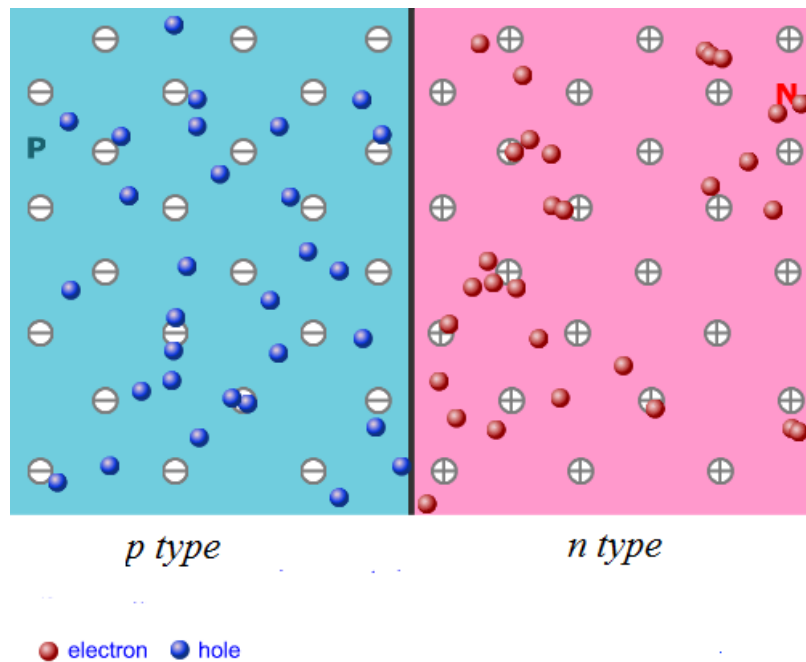
Fig.1.12. Schematic view of P-N junction [12].

A p-n junction can be used as a photodiode as the diode is sensitive to the light when the configuration of the diode is reverse biased. It can be used also as a solar cell. On the other hand, when the diode is forward biased, it can be used in LED lighting applications. One can use it also as rectifiers in many electric circuits and as a voltage-controlled oscillator in varactors [12].

1.5. Solar cells

If one applies light to a semiconductor; the electron-hole pairs might be excited if the photon energy is greater than the band gap energy. In most semiconductor regions, the created electrons and holes will rapidly separate. However, in the depletion region, due to the electric field in this region, the created electrons flow to the left (towards the n-doped region) and the holes created to the right (towards the p-doped region). In both cases, the charge current is moving to the right (negative flow left and positive flow to the right form a current flowing to the right). Thus a p-n junction automatically creates a current (and hence a voltage, and therefore a force) once exposed to light. Devices based on this principle, known as solar cells, photovoltaics, or photovoltaic cells, currently provide a huge electrical energy to the world [27].

1.5.1. Solar Cell Structure

A solar cell is an electronic device that converts sunlight directly into electricity. The bright light on the solar cell produces both current and voltage to generate electrical energy. This process requires first, a material in which the absorption of light raises the electron to a higher energy state, and second, the movement of this higher energy electron from the solar cell into an external circuit. Then the electron dissipates its energy in the outer circuit and returns to the solar cell. A variety of materials and processes can meet the requirements of photovoltaic conversion, but in practice, almost all photovoltaic conversion processes use semiconductor materials in the form of a p-n junction [12].
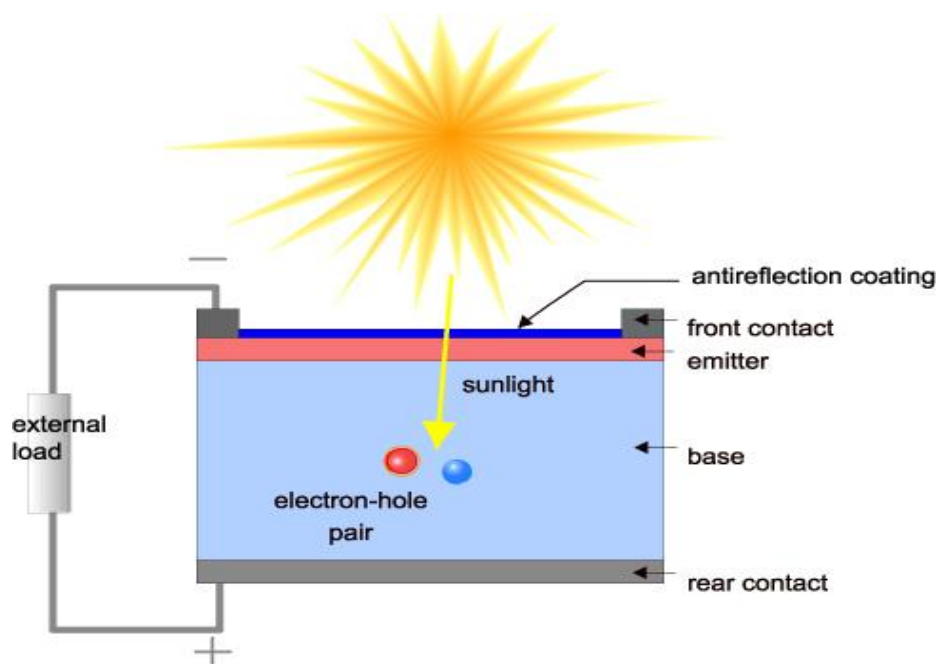
Fig.1.13. Cross section of a solar cell [12].

The basic steps in the operation of a solar cell are starting from the generation of light-generated carriers then a collection of the light-generated carries start generating a current resulting in a large voltage across the solar cell and the final step is the dissipation of power in the load and in parasitic resistances.

1.5.2. Light generated current

Generating current in a solar cell, known as "photocurrent", involves two main processes. The first process is the absorption of the incident photons into pairs of electronic holes. The electron-hole pairs will be generated in the solar cell on the condition that the incident photon has energy greater than the energy of the band gap. However, the electrons (in the p-type

material) and holes (in the n-type material) are stable above the plane and will only be present, on average, for a period of time equal to the lifetime of the minority holder before recombining. If the carrier is re-recombined, the light-generating electron-hole pair is lost and no current or energy can be generated. A second process, which is to collect these carriers via the p-n junction, prevents this recombination by using the p-n junction to separate the electron from the hole spatially. The carriers are separated by the electric field at the p-n junction. If the light-generated minority carrier reaches the p-n junction, it is traversed across the junction by the electric field at the junction, where it is now a majority conductor. If the emitter and the base of the solar cell are connected together (that is, if the solar cell is short-circuited) then the light-generating carriers flow through the external circuit [12].

1.5.3. The construction of the solar cell

The cell used in this work is built as indicated in the following figure 1 below [27]:
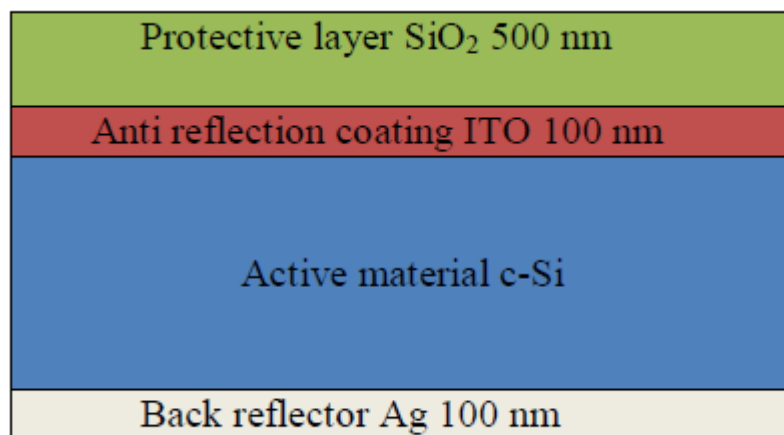
Fig.1.14. Structure of the solar cell used in the simulation [27].

It is composed of the following layers:

1-Protective layer: Its main objective is to protect the cell from the extern influences, like shocks, rain, rocks and it's of silicon dioxide SiO_2.

2-Anti reflecting coating ARC: It is used to minimize optical losses caused by reflection; recently this film is made of a transparent conducting oxide TCO used as ARC and a front electrode.

3-Active material: it can be made of crystalline silicon (c-Si) or amorphous one (a-Si). This layer absorbs light and generates the electron hole pairs. It can be depredated with time due light shining for a long period of time

4-Rear reflector: It can be made of silver (Ag) and it's ideally reflective to reflect light back to the active material, because it is considered as a mirror due to its free electrons, thus there is no transmittance in the cell [27].

The photovoltaic QCRF-FDTD simulator tool [28] allows us to calculate the important parameters of the indicated cell like (Jsc, Voc, FF, E_{ff}).

1.6. Conclusion

The main objective of this first chapter was to understand the interactions of light-matter which the principle of the solar cell function. At the end we showed the construction of the photovoltaic cell where the active layer can be a semiconductor like crystalline or amorphous silicon. The properties of this material are a key factor that determines the efficiency of the cell. In the following chapter, we are going to deal with light enhancement in the cell using surface refractive gratings or texturing. The idea behind this is reducing the thickness of the active layer and increasing the probability of the photons to be absorbed thus generating electron-hole pairs.

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Chapter 2

Light Trapping by Surface Gratings Diffraction

2.1. The surface of materials

Surface science is not an ancient science however; this term appeared way back in the early 1960s. Although lot of theoretical concepts have already been developed when they were studying some related phenomena [1].

The surface is the simplest case of the interface (contact between two surfaces from the same or different matter), at which the solid is in contact with the vicinity such as the vacuum and gas. The development of modern interface physics is mainly determined by the theoretical concepts and experimental tools that are being developed in the field of surface physics, that is, simple solid vacuum interface physics. In the meantime, surface physics itself has become an important branch of microscopic solid-state physics, although its historical roots lie in classical bulk solid-state physics and physical chemistry, particularly the study of surface interactions and heterogeneous catalysis [2].

The concepts of surface and interface physics are important in solid state physics, not only in relation to special experimental tools but also for specific physical systems. The rigid thin film deposited on the substrate is bound by a rigid solid interface and its surface (vacuum film interface). Thus the properties of this thin film are mainly determined by the properties of its two interfaces [2].

2.2. Surface texturing

Surface texture is a surface modification technique that intentionally changes the surface texture, in order to improve, among other things, its absorption performance. This is obtained through various patterns, which can be of micro or nano scale, created on the contact surfaces. The surface sealed performance depends on the shape, geometry, surface texture pattern, and operating condition of the contact components. There are a number of different techniques for surface texturing, among which surface fabric is often used with a laser. It can be performed either as a micro and nano asperities (protrusions) or micro and nano holes (dimples), Figure 2.01, with the latter being more popular [3].
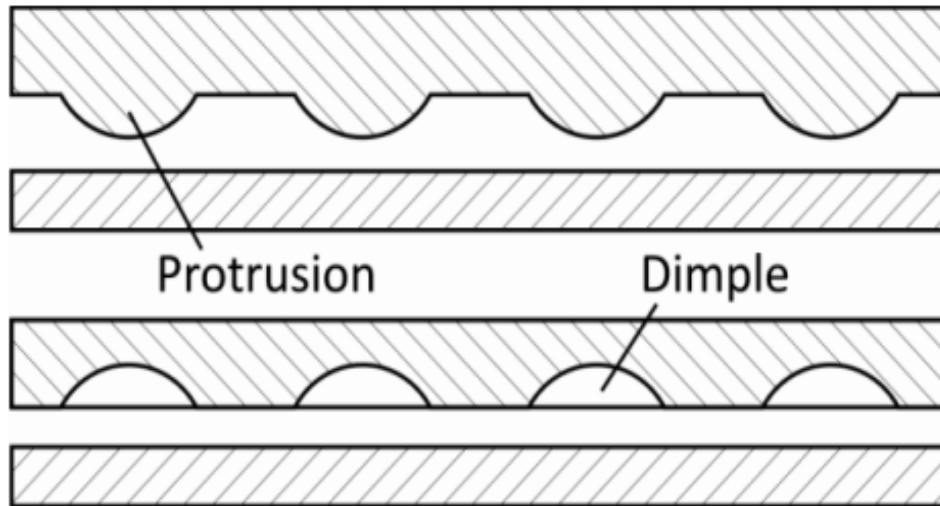
Fig. 2.01. Different principle of intentionally made surface texturing with some surface modification technique [3].

Inverted pyramid texturing is another type of surface texturing, where, the pyramids are drilled down into the silicon surface instead of being etched to indicate the top of the surface [4, 5]

Fig. 2.02. Scanning electron microscope photograph of a textured silicon surface. Image Courtesy of the School of Photovoltaic & Renewable Energy Engineering, University of New South Wales [6].

2.3. Surface gratings diffraction

The diffraction grating was firstly seen by James Gregory in 1673 when he shined a beam of light on a fine white feather. While the first man w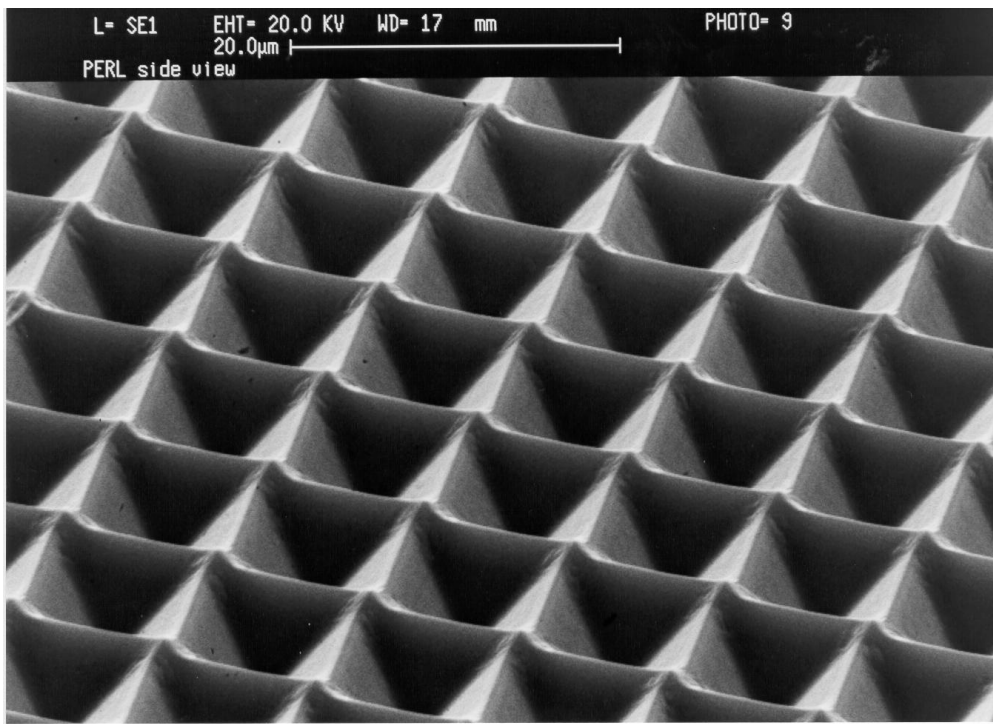ho really made the diffraction grating in 1785 using hair or thin wires evenly spaced across the threads of two parallel screws. This type of grating can be thought of as a linear, transmission grating very much like multiple slit diffraction configuration, where the hair blocks the light while the spacing between the hair acts like the slits [7].

A diffraction grating is a group of reflective (or transmitting) elements separated by a distance comparable to the wavelength of the studied light. It may be seen as a collection of reflective elements, such as a pattern of transparent slits (or openings) in an opaque screen, or a set of reflective grooves on a substrate (also called a blank). In both cases, the primary physical property of the diffraction grating is the spatial modification of the refractive index. Upon diffraction, the incident of an electromagnetic wave on a grating will modify its electric field amplitude, its phase, or both, in a predictable manner, due to the cyclic variation in the refractive index in the region near the surface of the grating.

The reflection grating consists of a grating as a reflective surface, while the transmission grating consists of a grating installed on a transparent surface.

The main grating (also called the original) is a network in which the surface relief pattern is created "from scratch", either by mechanical lining or 3D recording. A replica grating is one for which a surface relief pattern is created by casting or molding the relief pattern of another groove [8].

In 1821 Joseph von Fraunhofer rediscovered this technique and developed the equation relating the angle of diffracted orders to the grating spacing and wavelength of light [7].

2.3.1. Grating equation

When light is incident on a surface with a profile that is irregular at length scales comparable to the wavelength of the light, it is reflected and refracted at a microscopic level in many different directions as described by the laws of diffraction.

The two green beams represent the incident light on the binary lattice, after the reflection the light is deflected in many directions. We denote one of the rays as blue [9].
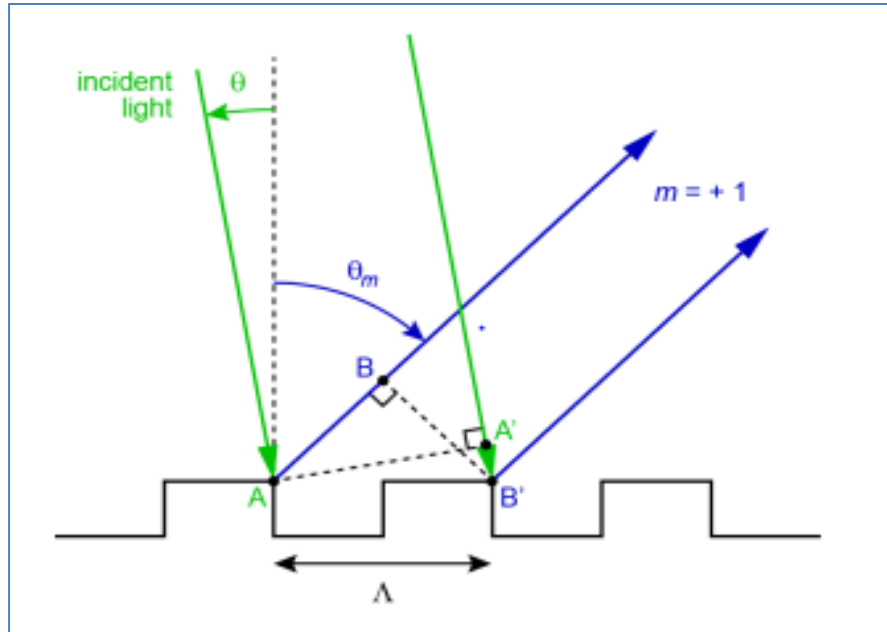
Fig. 2.03. Diagram showing path difference between rays scattered from adjacent rulings of reflective diffractive grating [9].

If the difference between adjacent green-blue ray paths diffracted off of identical locations on adjacent periods is equal to a multiple of the wavelength of light, the two blue rays interfere constructively.

Mathematically, the difference between paths AB and $A'B'$ is a multiple of the wavelength $m\lambda$;

$$AB - A'B' = m\lambda \qquad (2.01)$$

m : Diffraction order (integer)

λ : The wavelength of light

To find the difference paths of the two beams we have

$$\frac{AB}{\Lambda} = \cos(\frac{\pi}{2} - \theta_m) = \sin\theta_m \Rightarrow AB = \Lambda\sin\theta_m \qquad (2.02)$$

And

$$\frac{A'B'}{\Lambda} = \cos(\frac{\pi}{2} - \theta_i) = \sin\theta_i \Rightarrow A'B' = \Lambda\sin\theta_i \qquad (2.03)$$

The difference path equal to

$$AB - A'B' = \Lambda \sin \theta_m - \Lambda \sin \theta_i = m\lambda \qquad (2.04)$$

Rearranging the equation (2.04) we get the reflective grating equation given as follows.

$$\sin \theta_m = \sin \theta_i + m\frac{\lambda}{\Lambda} \qquad (2.05)$$

θ_m : The diffraction angle (°)

θ_i : The incident angle (°)

Λ : The period of the grating (nm)

For different media with different refractive indexes (n_1 and n_2) the equation (2.05) becomes

$$n1 \sin \theta_m = n2 \sin \theta_i + m\frac{\lambda}{\Lambda}$$

This relation is called grating equation which is very important in the following part where the period clearly appears in it. From this formula, it is clear that changing the period affects the angles and thus the path way of light.

To enhance the efficiency of the solar cell we need to trap the light inside the active layer of the solar cell. One of the most useful methods to trap the light inside the active layer is the gratings (putting peaks of nanocrystalline on the bottom of the active layer) as indicated in the figure 2.04 where the grating equation plays a crucial role.
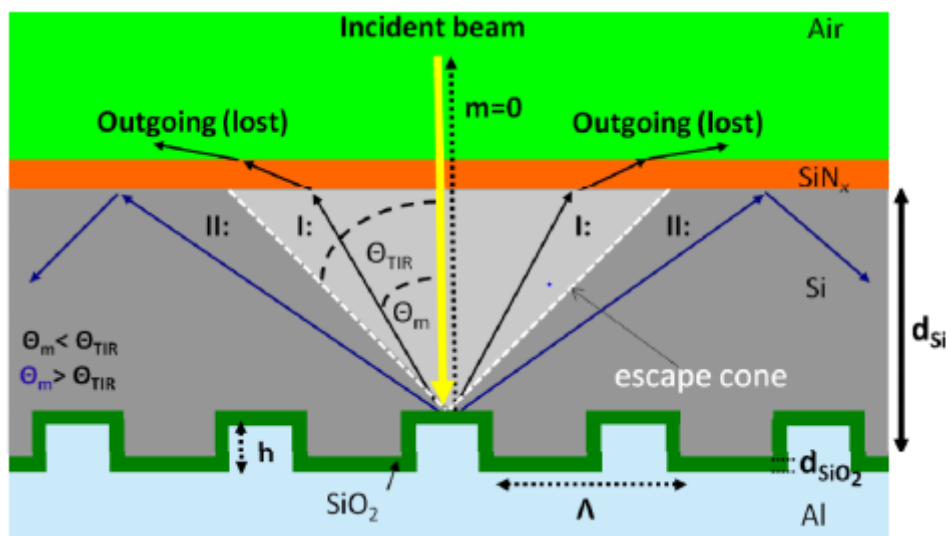

Fig. 2.04. Silicon solar cells structures with a backside grating [10].

2.3.2. The effect of the period Λ on the light trapping

The wavelength is one of the main characteristics of light. Thus, we should vary it in parallel with the period Λ using the equation below and see how it affects the diffraction angle [9]. If the first medium is air ($n1 \approx 1$) and the second medium is silicon ($n_2 = n_{si}$) so the grating equation becomes (2.06) bellow

$$\theta_m = \arcsin(\frac{\sin\theta_i}{n_{Si}} + m\frac{\lambda}{\Lambda n_{Si}}) \tag{2.06}$$
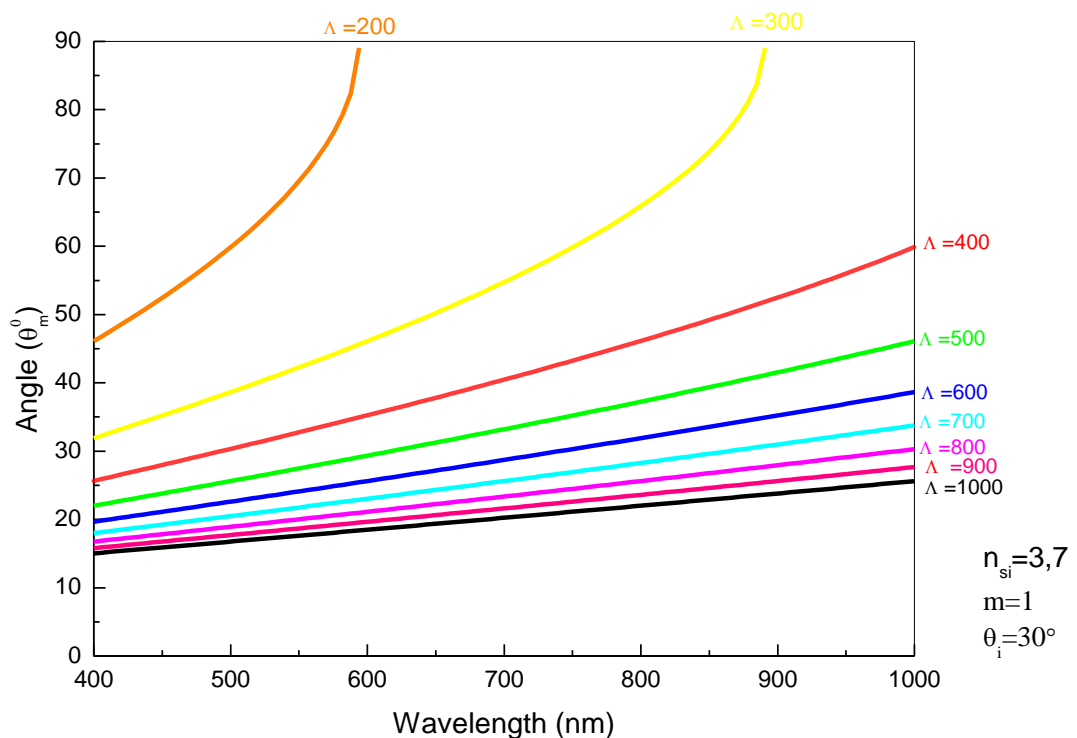
Fig. 2.05. The diffraction angle θ_m versus the wavelength in different cases of the period.

Figure 2.05 indicates that the shorter the period, the bigger angle of diffraction. However, the period 200 nm does not affect the entire light spectrum, thus the period should have a range between 300 and 400 nm.

Due to the fact which says: « the bigger the diffraction angle, the more amount of light trapped ». We tried to make it bigger by manipulating the period of the peaks on the bottom of the silicon active layer using the equation (2.06). We changed the period Λ a several different

ways and we saw the changes of θ_m by making the wavelengh, θ_i , n_{Si} and the order of diffraction m, constant.

Decreasing the period Λ with and ε each time is the first manner of varying the period as shown in (2.07) which illustrates that we start with a period and then we reduce it

$$\Lambda_0 = (\Lambda + (\Lambda - \varepsilon) + (\Lambda - 2\varepsilon) + (\Lambda - 3\varepsilon) + ... + (\Lambda - (\varepsilon n - 1))) / n \qquad (2.07)$$

Where ε is a constant small variation in the period (nm) and n is the order of the period. We replace (2.07) in (2.06) we can obtain the following results indicated by figure (2.06).
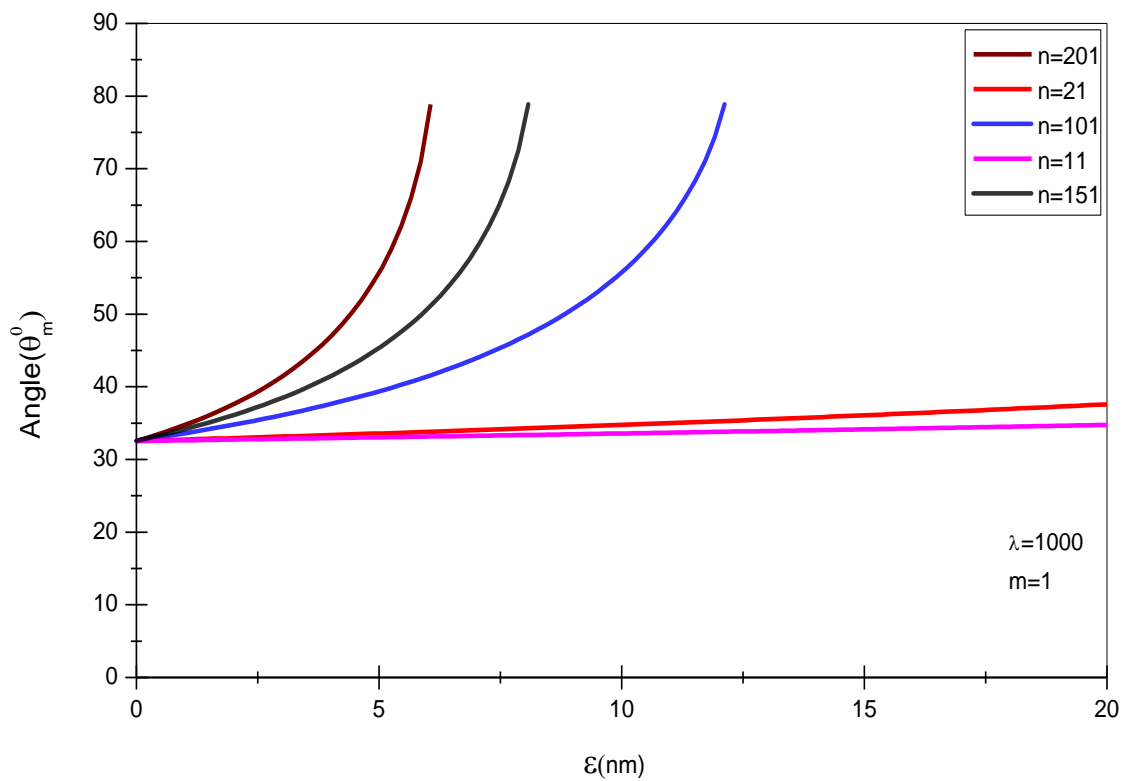
Fig. 2.06. The diffraction angle θ_m vs the change in the period ε .

From the plot above we see that all orders of period start from the same point. By increasing the change in the periods ε , we see that the higher order of period such as 151,101, 201, have a bigger diffraction angle than the lower orders of the period.

Now if we change the strategy by reducing and increasing the period between pillar gratings as indicated by the following equation:

$$\wedge_0 = \wedge + (\wedge - \wedge/2) + (\wedge + \wedge/3) + (\wedge - \wedge/4)......*1/n$$

if we replace this formula into (2.06) we can get the graph in figure 2.07 which strongly shows the effect of this type of variation. When the number (n) is bigger the (around 100) we get the same angle of incidence.
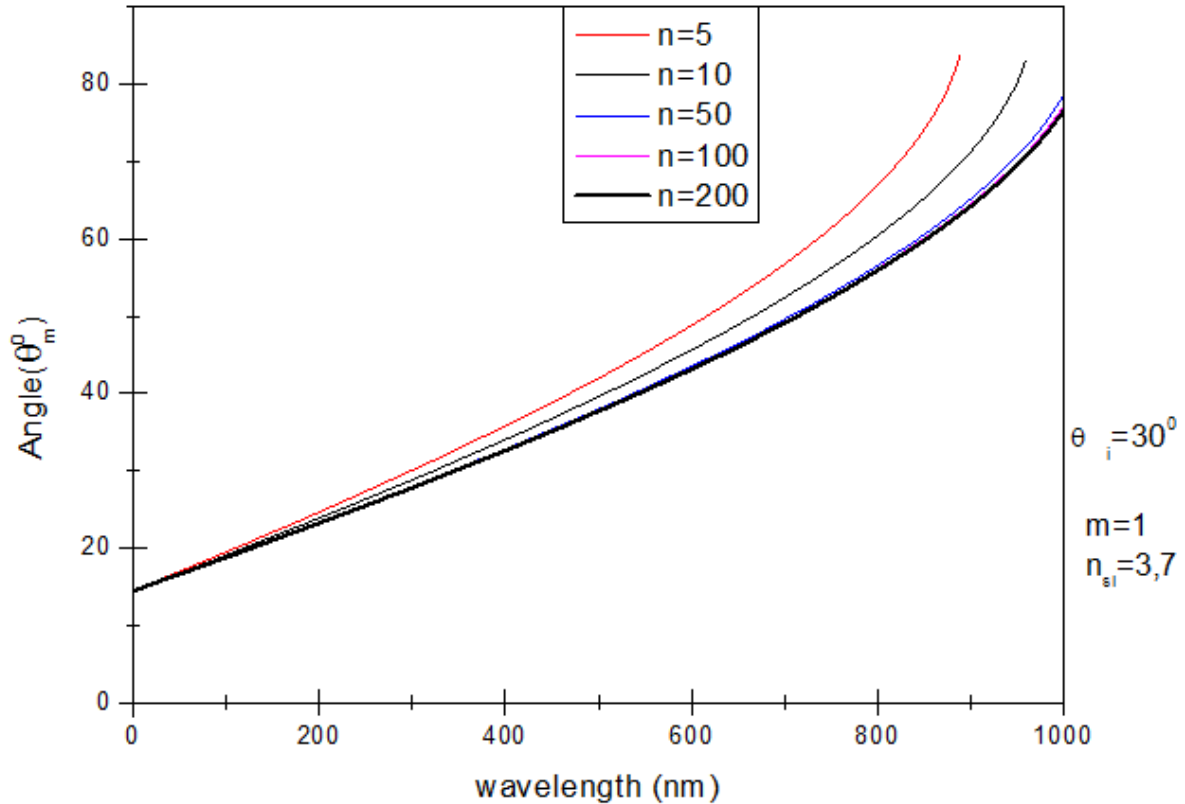
Fig. 2.07. The diffraction angle θ_m vs the change in the period by increasing and decreasing .

We did also some other calculation using this idea of changing the period like increasing it directly and the corresponding results are not indicated here

Changing the incident angle in parallel with the period is indicated in the figure 2.08 where we see that the increase in the diffraction angle corresponds with the increase in the incident one.
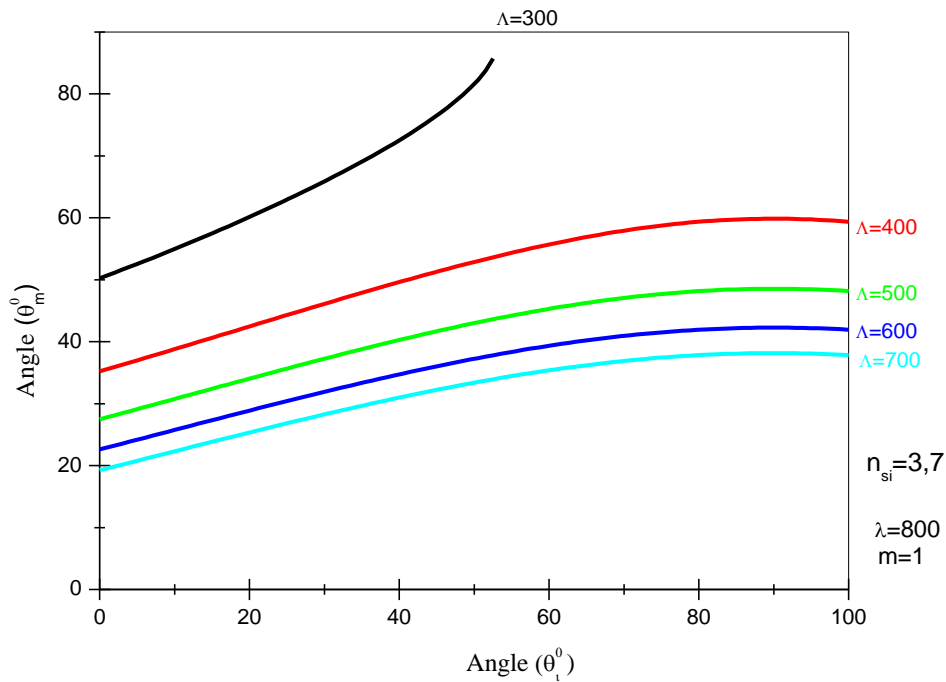
Fig. 2.08. Angle of incidence vs the angle of diffraction with changing the period.

It should be noted that the larger the period Λ, the more orders there are [9]. In general, the period should affect the entire spectrum of the light that means it should be ranging from 300 to 600 nm and the angle of incidence should be greater than $60°$ to $90°$.

In the active layer of solar cell, when creating the surface gratings diffraction using other material usually made of oxide layer so the whole mixture of the structure (active layer and the pillar) can be considered as a material of two phases named effective medium. How about the refractive index of this medium and its effect on the light trapping

2.3.3. The effective medium

Since the refractive index is one of the main factors that characterize the material. And we all know that the solar cell is a combination of several materials with different refractive indexes. Thus, the approximation of effective medium [11] has been proposed to study this kind of problem.

Several approximations have been used in the effective medium theory such as The Maxwell-Garnett approximation, Bruggeman approximation, Parallel model, Series model, Drude model [12].

In manuscript we are going to use the Drude model treating several different pair media such as: Si+ SiO_2, Si+TiO_2, Si+GaAs, Si+H_2O, Ge+SiO_2, H_2O+Si, TiO_2+GaAs.

Drude model (equation II.08) gives the effective refractive index in terms of the porosity and the refractive indices of the two different media [12].

$$n_{eff}^2 = (1-\varphi)n_a^2 + \varphi n_b^2 \tag{2.08}$$

Where n_a is the refractive index of the phase (a)

n_b is the refractive index of the phase (b)
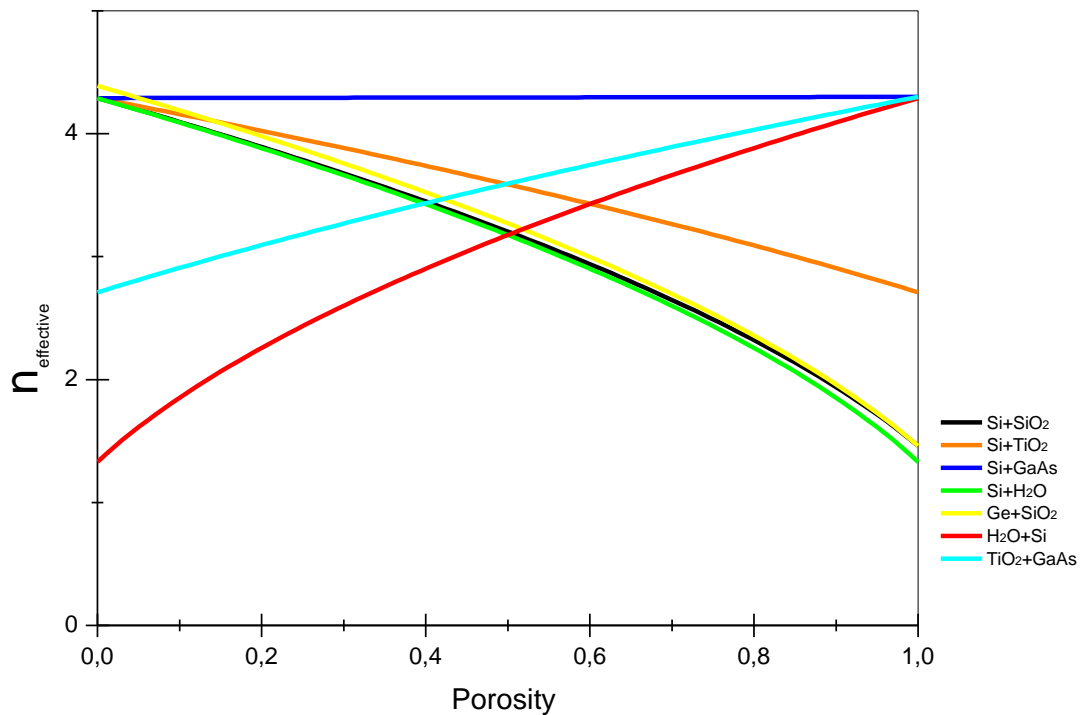
φ is the porosity.

Fig. 2.09. The effective refractive index vs the porosity.

Figure (2.09) indicates that when the refractive index of the media is close to equal the effective refractive index is a constant such as the case of the Si+GaAs.

In the cases of H_2O+Si and TiO_2+GaAs, the effective refractive index is increasing when the porosity is increased because the n of H_2O and TiO_2 is less than n of Si and GaAs, respectively.

When the refractive index of the medium (a) is greater than the medium (b), the effective refractive index is decaying in parallel with the increase of porosity in the cases of Si+ SiO_2 Si+TiO_2, Si+H_2O, Ge+SiO_2.

The effective refractive index may have a positive effect on the light trapping by changing the diffraction angle which is our main goal.

2.3.4. The evanescent field

"Evanescent" means "tend to disappear" which is convenient because the intensities of evanescent waves decay exponentially (not sinusoidally) with the distance from the interface at which they form as shown in figure 2.10. Evanescent waves are formed when sine waves are reflected (inwardly) at an interface at an angle greater than the critical angle (equation 2.09) so that the total internal reflection occurs [13].

$$\theta_c = \arcsin(\frac{n_2}{n_1}) \qquad\qquad (2.09)$$

Where θ_c is the critical angle, n_1 and n_2 are the refractive indices of the first and the second media respectively.

Investigation of the contribution of evanescent waves to the far-field has become of considerable interest in recent years because of its significance to near-field microscopy, high-density recording, and subwavelength lithography [14].
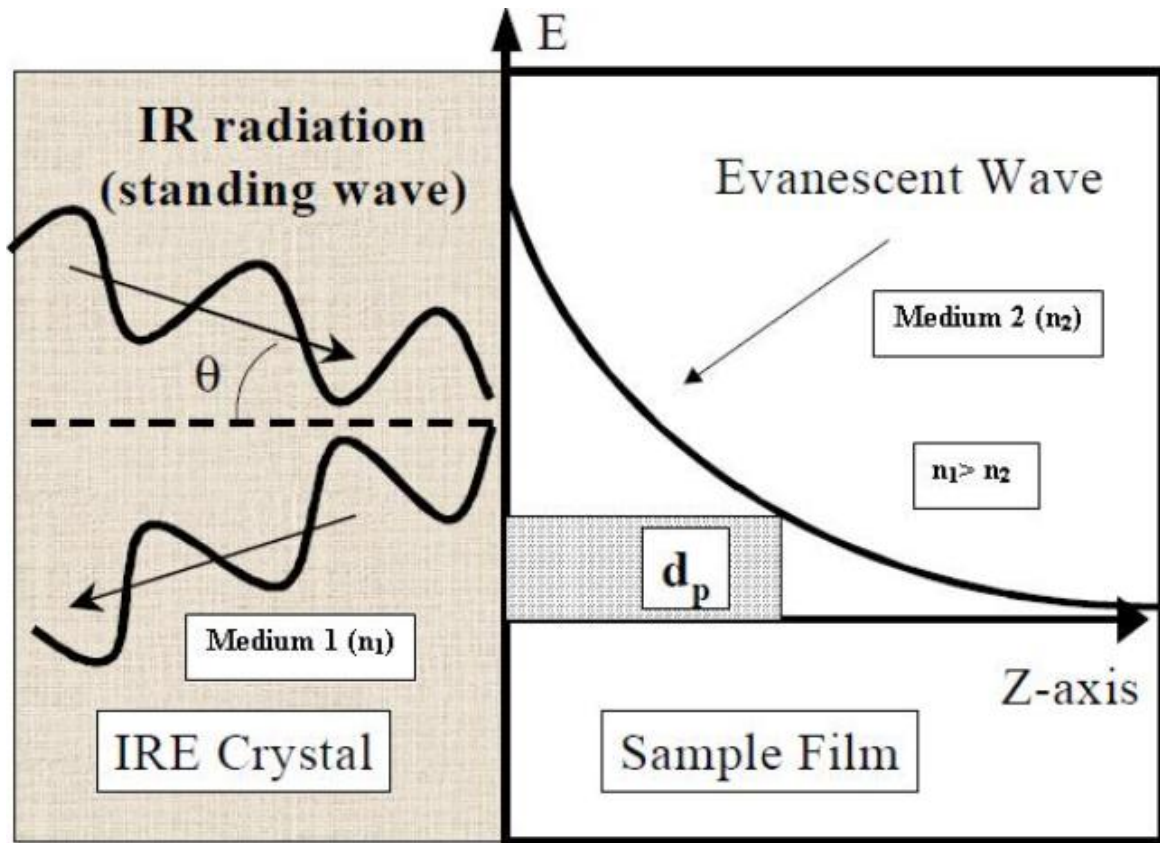
Fig. 2.10. Schematic of the evanescent wave formed at the internal reflection element sample surface. d_p is defined as the penetration depth [15].

The evanescent wave penetrates into the surrounding area and is sufficient to excite particles near the core. Penetration depth is a fraction of a wavelength if the incident light is perpendicular to the interface and can be extended to several wavelengths if the angle of incidence is at the critical angle. The depth of penetration is determined by (d_p) [16] :

$$d_p = \frac{\lambda}{2\pi n_1 (\sin^2(\theta_i) - \frac{n_2^2}{n_1^2})^{1/2}} \tag{2.10}$$

At small angles, the scattering of light at the lining interface is sinusoidal with a certain period. As the angle of incidence increases and approaches the critical angle, the period becomes longer and the light is scattered approximately parallel to the interface. At an angle of incidence coinciding with the critical angle, the wave period becomes infinite and the refracted light wave fronts are aligned perpendicular to the interface.

In this work, we tried to measure the penetration depth in the cases indicated in the figure below.
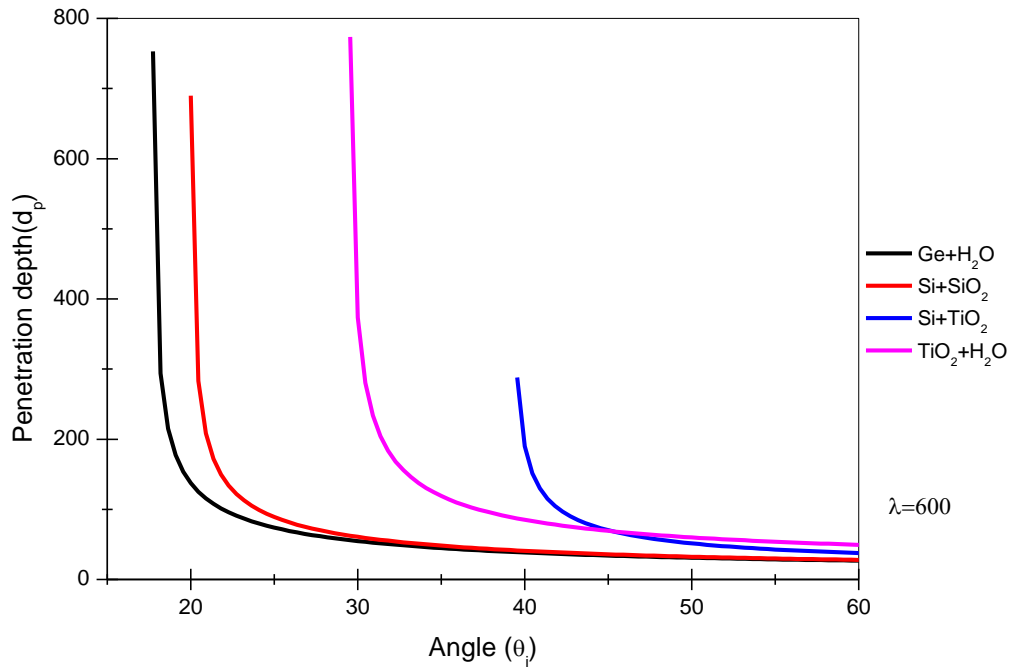
Fig. 2.11. The penetration depth d_p(nm) in terms of the incidence angle.

Figure 2.11 tells us that the penetration depth has the same pattern with all cases; the maximum value of the (d_p) is right on the critical angle and it is decaying exponentially with the increase of the incident angle. But the maximum and the minimum value differs from one case to another as we see in the plot above. Since the characterization of the apertured fiber probe and the near-field interactions of the silver nanocluster are two typical examples of the applications of the evanescent field of TIR. Furthermore, the evanescent wave (field) is very sensitive to the variations of the morphology and optical properties of the interface [17]. Thus, its penetration is one of its properties to enhance the efficiency of its applications.

2.4. Conclusion

From this chapter and the results indicated we learnt that trapping light is very important due to its application in solar cell which may be the future of the world in term of energy. Trapping light can be done by surface texturing or surface refractive gratings where the period plays a crucial role in this way.

We thought to change slightly the period of gratings to enhance light and this was clearly shown by the results we chose to report here.

When putting refractive gratings this means changing the structure thus the medium is named effective one and the refractive index changes this is the reason behind indicating the theory

of effective media and determine its refractive index that is important the equation of gratings well discussed in the beginning of this chapter.

As we indicated the enhancement of light is based on the total reflexion and at the point of this rellexion we have an evanescent field with a penetration depth that can be used to characterize surface adsorpted molecules in other techniques such as attenuated total reflexion spectroscopy (ATR-FTIR).

We clearly showed is this part the importance of light trapping and the corresponding equation plus the structure of the cell becomes.

II.5.References

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General conclusion

A surface diffractive grating is a suitable and a good method used in light trapping inside the solar cell to increase its path. Thus the probability of light for being absorbed will automatically be increased. The period between the pillars is very important and should not be very small or very big compared to the light we are looking to trap. The strength point of this method is giving the possibility of using a thin active layer but with a high efficiency compared to other layer without diffractive gratings.

According to our personal imagination by using a surface with different geometries base on the different periods between pillar diffractive gratings, we indicated that light can be trapped differently and strongly depends on the period and the way of changing this period. This phenomenon is formulated by the grating equation and one of the most important parameter is the refractive index of the materials and that is why we tried to deal with the theory of effective medium which is a mixture of two or more different materials. We showed the effective refractive index of two phases. To conclude this simple work based on the total reflexion of light, we tried to understand another important parameter which the evanescent field at the point of total reflexion where the angle of incidence, the wave length and the refractive index are dominant parameters in determining the penetration depth.

As future recommendations, we may think about using two different forms of diffractive gratings with different periods. It is possible also to imagine the pillars like holes inside the layer and not outside as we reported here.

At the end, it is very important to mention that the position of our country, Algeria, in the globe is very interesting and we have a huge desert where we can use solar energy for electricity to safe the fossil one for next generation. It is our duty as researchers to think about the most important solutions in this field and this gives the present project a real value so I wish that we can do more in term of research in the future to improve this field.