To Study the Confinement and Energy States of III-V Semiconductor based Quantum Well Solar Cell

EAST WEST UNIVERSITY

Department of Electronics and Communication Engineering

Thesis title

To Study the confinement and energy states of III-V Semiconductor based Quantum Well Solar Cell

Supervisor

Dr. Nahid Akhter Jahan

Assistant Professor

Department of Electronics and Communication Engineering

Submitted by

Md. Shahriar

Id: 2012-2-55-047

Monayem Khan

Id: 2012-2-55-011

Declaration

This report on the basis of our thesis paper and its enhancement of studies throughout our thesis work is submitted to follow the terms and condition of the department of electronics and communications engineering .This report is the requirement for the successive competition of B.Sc engineering in Electronics and communication engineering.

We state that the report along with its literature that has been demonstrated in this report papers, is our own work with the masterly guidance and fruitful assistance of our supervisor for the finalization of our report successfully.

Signature: signature:

-------------------------------   ------------------------ -

Md. Shahriar   **Monayem Khan**

ID: 2012-2-55-047   **ID: 2012-2-55-011**

Signature of supervisor :	Signature of chairpersons :
-- Dr. Nahid Akhter Jahan Phd Assistant Professor, Department of Electronics and communications engineering, East West university. Dhaka, Bangladesh.	--- Dr.M.Mofazzal Hossain Phd Professor, Department of Electronics and communications engineering, East West university. Dhaka, Bangladesh

Acknowledgement

Incipiently, we would like to express our profound gratitude and deep regards to Dr. Nahid Akter Jahan for his guidance and invariable support throughout the project effort. we have successfully accomplished the goal of the project due to him tireless and patient monitoring during the time of our thesis .we are extremely grateful to him as he gives as the opportunity and exposure that we never would have had if he had not worked with us.

We also so pleased to all our faculty members of ECE department for their guidance and support for successive completion of our graduation degree. Similarly, we would like to thanks our friends who help us to make this thesis paper.

We would like to pay our homage to our parents whose encouragement and prayer are always with us and moving with us like a shadow of mine which will protect us in any emergency situation. The name without whom our thanksgiving is incomplete is the almightily Allah, who allowed us to live in this beautiful worlds.

Thanks you all for your grate support to us.

Approval

This project report "the confinement and energy states of III-V Semiconductor based Quantum Well/Dot Solar Cell " submitted by Md.Shahriar , ID: 2012-2-55-047 and Monayem khan , ID: 2012-2-55-011 to department of Electronics and Communication Engineering. East West University has been accepted as satisfactory for the partial fulfillment of the requirements for the degree of Bachelor of Science in Electronics and Communication Engineering and approved as to its style and contents.

Approved By:

Supervisor

Dr.Nahid Akter Jahan,Phd

Assistant Professor,

Department of Electronics and Communication Engineering,

East West University.

Abstract

A **quantum Well Solar Cell** is a solar cell design that uses quantum dots/well as the absorbing photovoltaic material. Quantum Well (QW) solar cells have the potential to increase the maximum attainable thermodynamic conversion efficiency of solar photon conversion up to about 66% by utilizing hot photo generated carriers to produce higher photo voltages or higher photocurrents. The main advantage with quantum dots is the ability to tune the size of the dots for many applications. Their electronic characteristics are closely related to the size and shape of the individual crystals. In this work we have investigated four different configuration QW heterostructures including both bunary and ternary semiconductors such as InAs/GaAs, InSb/GaSb, AlGaSb/InGaSb and AlGaAs/InAs.

Table of Contents

Chapter 1

Fundamentals of Semiconductor

1.1 Introduction:

Solar cell is P-V junction semiconductor device. In order to understand the design and operation of solar cells, it is important to understand the fundamentals of semiconductors. Semiconductor in solar cell applications are discussed the distribution of electrons in various orbits in an atom, energy band gap of various semiconductors etc.

1.2 Semiconductor:

A semiconductor is a substance, usually a solid chemical element or compound, that can conduct electricity under some conditions but not others, making it a good medium for the control of electrical current. Its conductance varies depending on the current or voltageapplied to a control electrode, or on the intensity of irradiation by infrared (IR), visible light, ultraviolet (UV), or X rays. The specific properties of a semiconductor depend on the impurities, or *dopants*, added to it. An *N-type* semiconductor carries current mainly in the form of negatively-chargedelectrons, in a manner similar to the conduction of current in a wire. A *P-type*semiconductor carries current predominantly as electron deficiencies called holes. A hole has a positive electric charge, equal and opposite to the charge on an electron. In a semiconductor material, the flow of holes occurs in a direction opposite to the flow of electrons.[1]

1.3 Properties of semiconductor:

1.3.1 Variable conductivity

Semiconductors in their natural state are poor conductors because a current requires the flow of electrons, and semiconductors have their valence bands filled, preventing the entry flow of new electrons. There are several developed techniques that allow semiconducting materials to behave like conducting materials, such as doping or gating. These modifications have two outcomes: n-type and p-type. These refer to the excess or shortage of electrons, respectively. An unbalanced number of electrons would cause a current to flow through the material.

1.3.2 Heterojunctions

Heterojunctions occur when two differently doped semiconducting materials are joined together. For example, a configuration could consist of p-doped and n-

dopedgermanium. This results in an exchange of electrons and holes between the differently doped semiconducting materials. The n-doped germanium would have an excess of electrons, and the p-doped germanium would have an excess of holes. The transfer occurs until equilibrium is reached by a process called recombination, which causes the migrating electrons from the n-type to come in contact with the migrating holes from the p-type. A product of this process is charged ions, which result in an electric field.

1.3.3 Excited Electrons

A difference in electric potential on a semiconducting material would cause it to leave thermal equilibrium and create a non-equilibrium situation. This introduces electrons and holes to the system, which interact via a process called am bipolar diffusion. Whenever thermal equilibrium is disturbed in a semiconducting material, the amount of holes and electrons changes. Such disruptions can occur as a result of a temperature difference or photons, which can enter the system and create electrons and holes. The process that creates and annihilates electrons and holes are called generation and recombination.

1.3.4 Light emission

In certain semiconductors, excited electrons can relax by emitting light instead of producing heat. These semiconductors are used in the construction of light emitting diodes and fluorescent quantum dots.

1.3.5 Thermal energy conversion

Semiconductors have large thermoelectric power factors making them useful in thermoelectric generators, as well as high thermoelectric figures of merit making them useful in thermoelectric coolers.[2]

1.4 Construction and Working principle of solar cell:

Various materials display varying efficiencies and have varying costs. Materials for efficient solar cells must have characteristics matched to the spectrum of available light. Some cells are designed to efficiently convert wavelengths of solar light that reach the Earth surface. However, some solar cells are optimized for light absorption beyond earth's atmosphere as well. Light absorbing materials can often be used in multiple physical configurations to take advantage of different light absorption and charge separation mechanisms. Many currently available solar cells are made from bulk

materials that are cut into wafers between 180 to 240 micrometers thick that are then processed like other semiconductors. Other materials are made as thin-films layers, organic dyes, and organic polymers that are deposited on supporting substrates. A third group are made from nanocrystals and used as quantum dots (electron confined nanoparticles). Silicon remains the only material that is well-researched in both bulk and thin-film forms.

The solar cell works in three steps:

1) Photons in sunlight hit the solar panel and are absorbed by semiconducting materials, such as silicon.

2) Electrons (negatively charged) are knocked loose from their atoms, causing an electric potential difference. Current starts flowing through the material to cancel the potential and this electricity is captured. Due to the special composition of solar cells, the electrons are only allowed to move in a single direction.

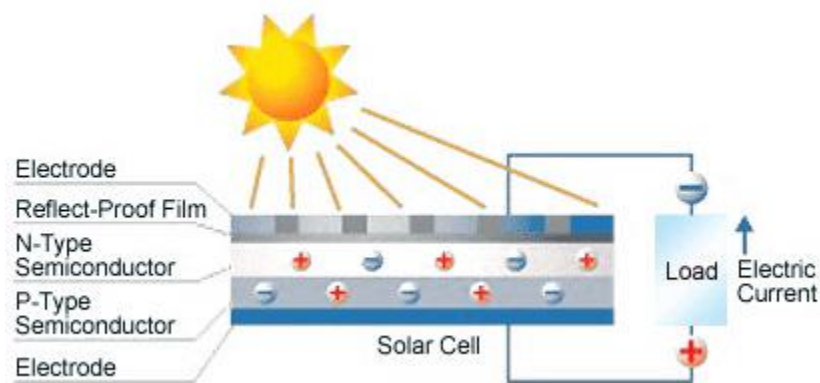3) An array of solar cells converts solar energy into amusable amount of direct current (DC) electricity.

Fig 1.1: Structure of Solar cell

1.6 Advantages of Solar Cell

1. No pollution associated with it.
2. It must last for a long time.
3. No maintenance cost.

Chapter 2

Types of solar cell

2.1 Introduction:

Solar cells are typically named after the semiconducting material they are made of. These materials must have certain characteristics in order to absorb sunlight. Some cells are designed to handle sunlight that reaches the Earth's surface, while others are optimized for use in space. Solar cells can be made of only one single layer of light-absorbing material (single-junction) or use multiple physical configurations (multi-junctions) to take advantage of various absorption and charge separation mechanisms.

2.2 Photovoltaic generation:

Solar cell divided into three main catagories called generation

2.2.1 1st generation solar cell:

The first generation cells—also called conventional, traditional or wafer-based cells—are made of crystalline silicon, the commercially predominant PV technology that includes materials such as poly silicon and mono crystalline silicon.
"First generation" panels include silicon solar cells. They are made from a single silicon crystal (mono-crystalline), or cut from a block of silicon that is made up of many crystals (multi-crystalline - shown at right).

2.2.2 2nd generation solar cell:

Second generation cells are thin film solar cells, that include amorphous silicon, CdTe and CIGS cells and are
Commercially significant in utility-scale photovoltaic power stations, building integrated photo voltaic or in small standalone power system.
"Second generation" thin-film solar cells are less expensive to produce than traditional silicon solar cells as

They require a decreased amount of materials for construction. The thin-film PV cells are, just as the name implies, a physically thin technology that has been applied to photovoltaics. They are only slightly less efficient than other types but do require more surface area to generate the same amount of power.

2.2.3 3rd generation solar cell:

The third generation of solar cells includes a number of thin-film technologies often described as emerging photo voltaic most of them have not yet been commercially applied and are still in the research or development phase.[3]
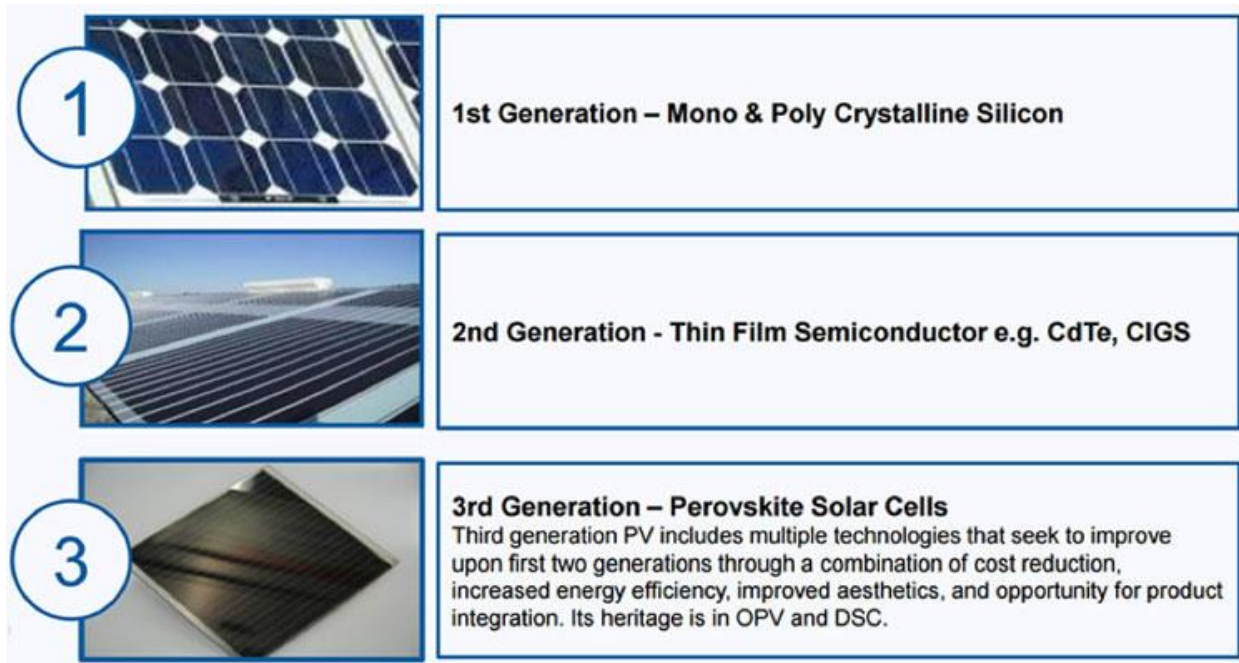

Fig 2.1: Generation of solar cell

2.3 Type of solar cell:

A solar cell (also called photovoltaic cell or photoelectric cell) is a solid state electrical device that converts the energy of light directly into electricity by the photovoltaic effect. The following are the different types of solar cells.

*Amorphous Silicon solar cell (a-Si)

*Cadmium telluride solar cell (CdTe)

*Concentrated PV cell (CVP and HCVP)

*Crystalline silicon solar cell (c-Si)

*Gallium arsenide germanium solar cell (GaAs)

*Hybrid solar cell

*Multi-junction solar cell (MJ)

*Organic solar cell (OPV)

*Plastic solar cell

*Polycrystalline solar cell (multi-Si)

*Polymer solar cell

*Quantum dot solar cell

*Solid-state solar cell

*Wafer solar cell, or wafer-based solar cell (synonym for crystalline silicon solar cell)

In this chapter we discussed about some of these types of solar cell.[4]

2.3.1 Amorphous Silicon solar cell (a-Si):

Amorphous silicon (**a-Si**) is the non-crystalline form of silicon used for solar cells and thin-film transistors in LCD displays.

Used as semiconductor material for **a-Si solar cells**, or **thin-film silicon solar cells**, it is deposited in thin films onto a variety of flexible substrates, such as glass, metal and

plastic. Amorphous silicon cells generally feature low efficiency, but are one of the most environmentally friendly photovoltaic technologies, since they do not use any toxic heavy metals such as cadmium or lead.
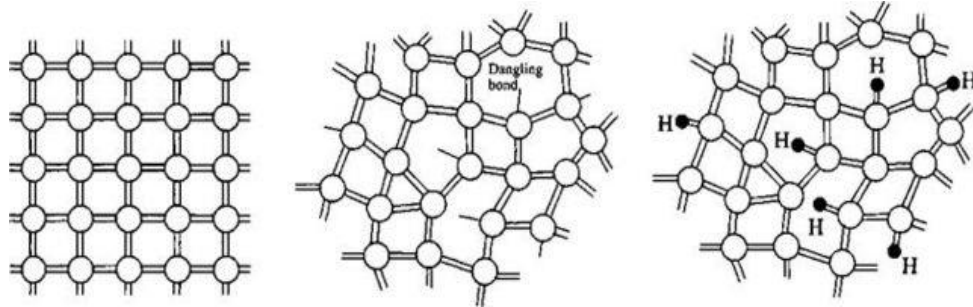

Fig 2.2: Amorphous Silicon (a-Si)

As a second-generation thin-film solar cell technology, amorphous silicon was once expected to become a major contributor in the fast-growing worldwide photovoltaic market, but has since lost its significance due to strong competition from conventional crystalline silicon cells and other thin-film technologies such as CdTe and CIGS.

Amorphous silicon differs from other allotropic variations, such as mono crystalline silicon—a single crystal, and poly crystalline silicon, that consists of small grains, also known as crystallites.[5]

2.3.1 Cadmium telluride solar cell (CdTe):

Cadmium telluride (**CdTe**) **photovoltaic's** describes a photovoltaic (PV) technology that is based on the use of cadmium telluride, a thin semiconductor layer designed to absorb and convert sunlight into electricity. Cadmium telluride PV is the only thin film technology with lower costs than conventional solar cells made of crystalline silicon in multi-kilowatt systems. On a lifecycle basis, CdTe PV has the smallest carbon footprint, lowest water use and shortest energy payback time of all solar technologies. CdTe's energy payback time of less than a year allows for faster carbon reductions without short-term energy deficits.
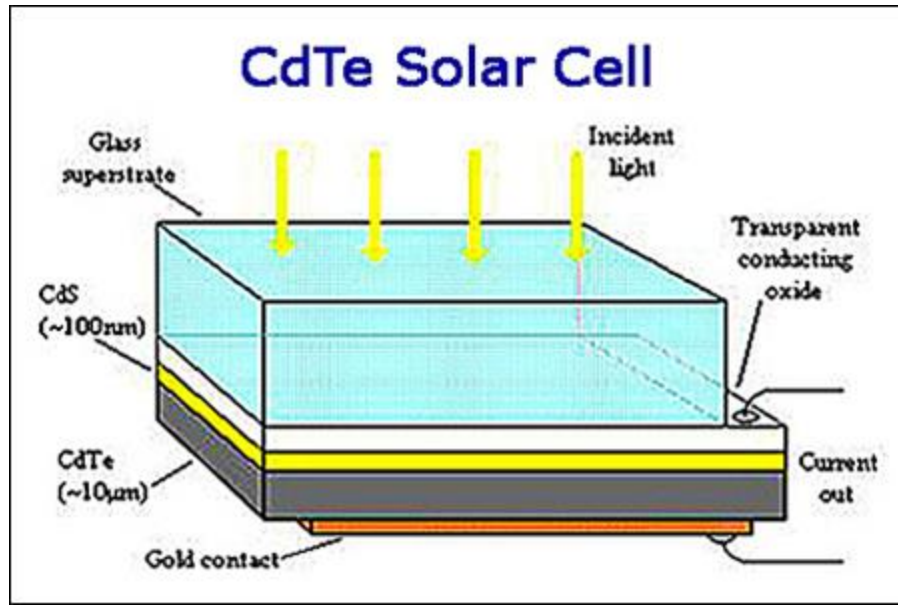
Fig 2.3: Cadmium telluride solar cell (CdTe)

2.3.2 Concentrated PV cell (CVP and HCVP):

Concentrator photovoltaic (**CPV**) is a photovoltaic technology that generates electricity from sunlight. Contrary to conventional photovoltaic systems, it uses lenses and curved mirrors to focus sunlight onto small, but highly efficient, multi-junction (MJ) solar cells. In addition, CPV systems often use solar trackers and sometimes a cooling system to further increase their efficiency. Ongoing research and development is rapidly improving their competitiveness in the utility-scale segment and in areas of high solar isolation. This sort of solar technology can be thus used in smaller areas.

Fig 2.4: Concentrated PV cell (CVP and HCVP)

2.4 Solar cell characteristic

2.4.1 Introduction:

Solar energy in one form or another is the source of nearly all energy on the earth. Humans, like all other animals and plants, rely on the sun for warmth and food. However, people also harness the sun's energy in many other different ways. For example, fossil fuels, plant matter from a past geological age, is used for transportation and electricity generation and is essentially just stored solar energy from millions of years ago. Similarly, biomass converts the sun's energy into a fuel, which can then be used for heat, transport or electricity. Wind energy, used for hundred of years to provide mechanical energy or for transportation, uses air currents that are created by solar heated air and the rotation of the earth. Photovoltaic's (often abbreviated as PV) is a simple and elegant method of harnessing the sun's energy. PV devices (solar cells) are unique in that they directly convert the incident solar radiation into electricity, with no noise, pollution or moving parts, making them robust, reliable and long lasting.

[18]

2.5 Parameters of solar cell:

Several important parameters which are used to characterize solar cells

1. Short circuit current
2. Open circuit voltage
3. Fill factor
4. Efficiency

1. Short circuit current:

The short-circuit current is the current through the solar cell when the voltage across the solar cell is zero (i.e., when the solar cell is short circuited). Usually written as I_{SC}, the short-circuit current is shown on the IV curve below.

The short-circuit current is due to the generation and collection of light-generated carriers. For an ideal solar cell at most moderate resistive loss mechanisms, the short-circuit current and the light-generated current are identical. Therefore, the short-circuit current is the largest current which may be drawn from the solar cell.

The short-circuit current depends on a number of factors which are described below:

- **The area of the solar cell.** To remove the dependence of the solar cell area, it is more common to list the short-circuit current **density** (J_{sc} in mA/cm^2) rather than the short-circuit current;
- **The number of photons** (i.e., the power of the incident light source). Isc from a solar cell is directly dependant on the light intensity as discussed in Effect of Light Intensity;
- **The spectrum of the incident light.** For most solar cell measurement, the spectrum is standardized to the AM1.5 spectrum;
- **the optical properties** (absorption and reflection) of the solar cell (discussed in Optical Losses); and
- **the collection probability** of the solar cell, which depends chiefly on the surface passivation and the minority carrier lifetime in the base

[19]
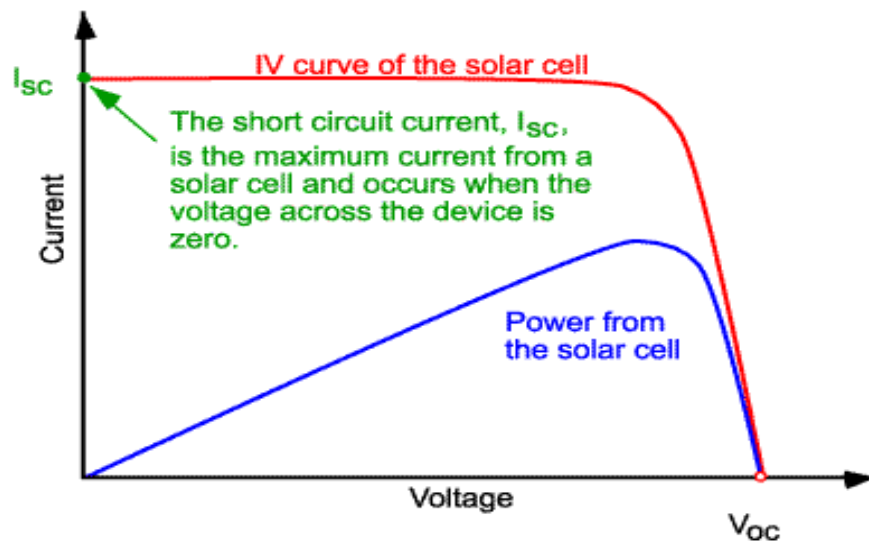
Fig 2.5: IV curve of a solar cell showing the short-circuit current

When comparing solar cells of the same material type, the most critical material parameter is the diffusion length and surface passivation. In a cell with perfectly passivity surface and uniform generation, the equation for the short-circuit current can be approximated as:

$$J_{SC} = qG(L_n + L_p)$$

………………………………. (2.1)

where G is the generation rate, and L_n and L_p are the electron and hole diffusion lengths respectively.

Silicon solar cells under an AM1.5 spectrum have a maximum possible current of 46 mA/cm^2. Laboratory devices have measured short-circuit currents of over 42 mA/cm^2, and commercial solar cell have short-circuit currents between about 28 mA/cm^2 and 35 mA/cm^2.
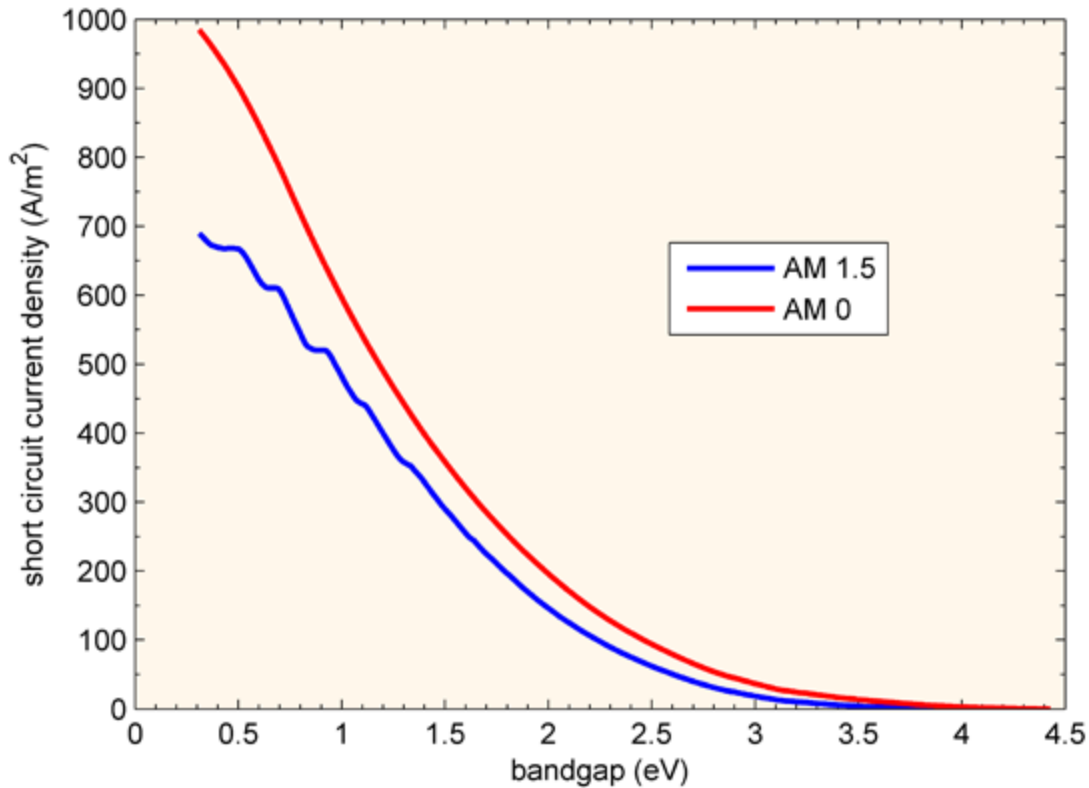
Fig 2.6: In an ideal device every photon above the band gap gives one charge carrier in the external circuit so the highest current is for the lowest band gap.

2. Open Circuit Voltage:

The open-circuit voltage, V_{OC}, is the maximum voltage available from a solar cell, and this occurs at zero current. The open-circuit voltage corresponds to the amount of forward bias on the solar cell due to the bias of the solar cell junction with the light-generated current. The open-circuit voltage is shown on the IV curve below.
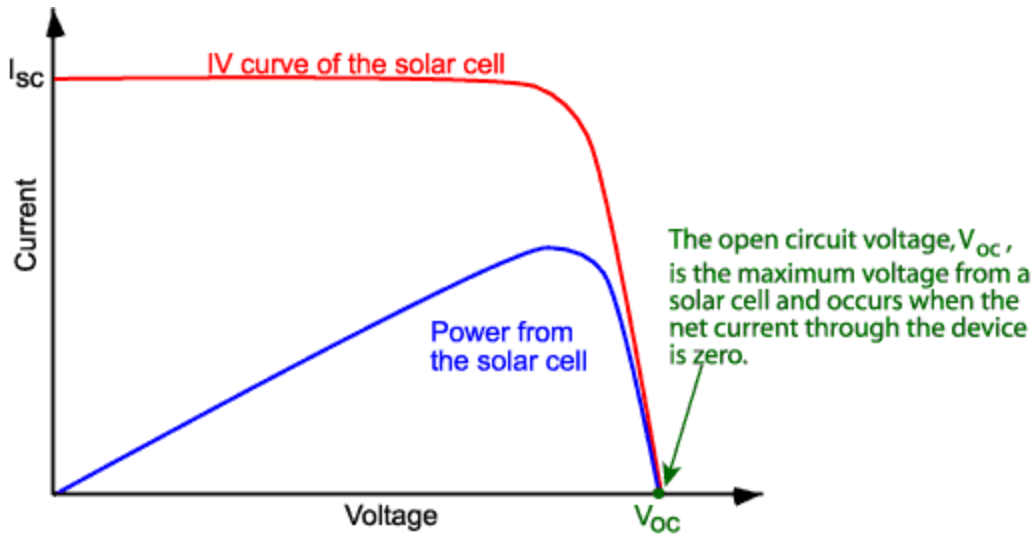
Fig 2.7: IV curve of a solar cell showing the open-circuit voltage.

An equation for V_{oc} is found by setting the net current equal to zero in the solar cell equation to give:

$$V_{OC} = \frac{nkT}{q} \ln\left(\frac{I_L}{I_0} + 1\right)$$

.... (2.2)

The V_{OC} can also be determined from the carrier concentration

$$V_{oc} = \frac{kT}{q} \ln\left[\frac{(N_A + \Delta n)\Delta n}{n_i^2}\right]$$

.... (2.3)

Where kT/q is the thermal voltage, N_A is the doping concentration, Δn is the excess carrier concentration and n_i is the intrinsic carrier concentration. The determination of V_{OC} from the carrier concentration is also termed Implied V_{OC}.

Where the short-circuit current (I_{SC}) decreases with increasing band gap, the open-circuit voltage increases as the band gap increases. In an ideal device the V_{OC} is limited by radioactive recombination and the analysis uses the principle of detailed balance to determine the minimum possible value for J_0.

The minimum value of the diode saturation current is given by:

$$J_0 = \frac{q}{k}\frac{15\sigma}{\pi^4}T^3 \int_u^\infty \frac{x^2}{e^x - 1}dx$$

................................(2.4)

where q is the electronic charge, σ is the Stefan–Boltzmann constant, k is Boltzmann constant, T is the temperature and

$$u = \frac{E_G}{kT}$$ ....(2.5)

Evaluating the integral in the above equation is quite complex. The graph below uses the method
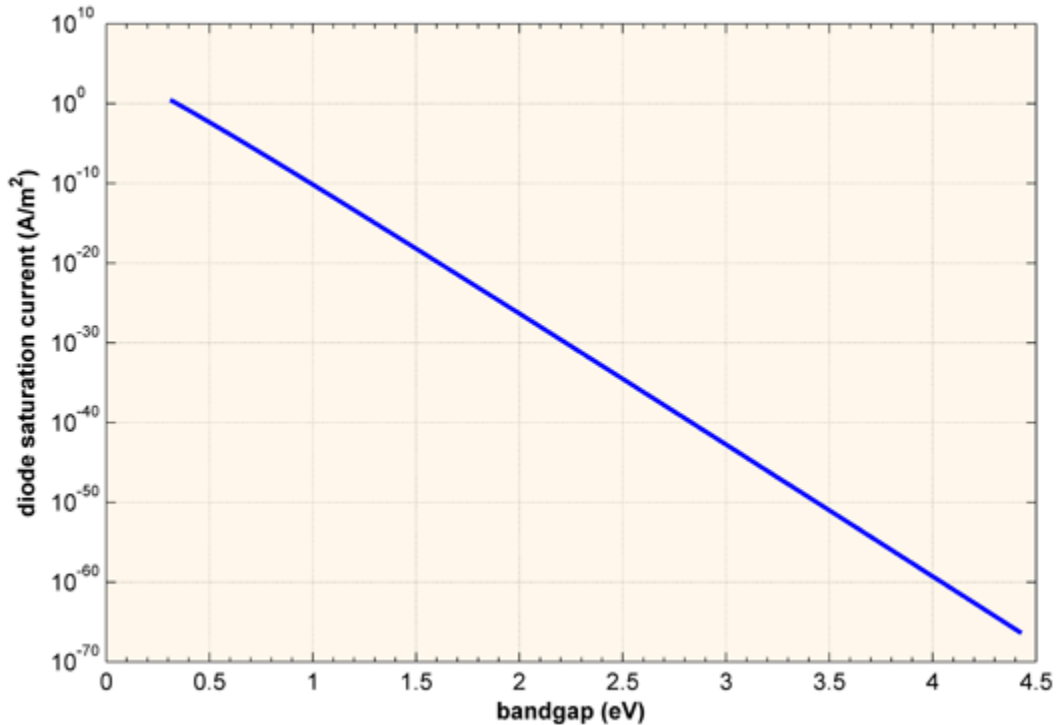
Fig 2.8: Diode saturation current as a function of band gap. The values are determined from detailed balance and place a limit on the open circuit voltage of a solar cell.

The J_0 calculated above can be directly plugged into the standard solar cell equation given at the top of the page to determine the V_{OC} so long as the voltage is less than the band gap, as is the case under one sun illumination.

[23]
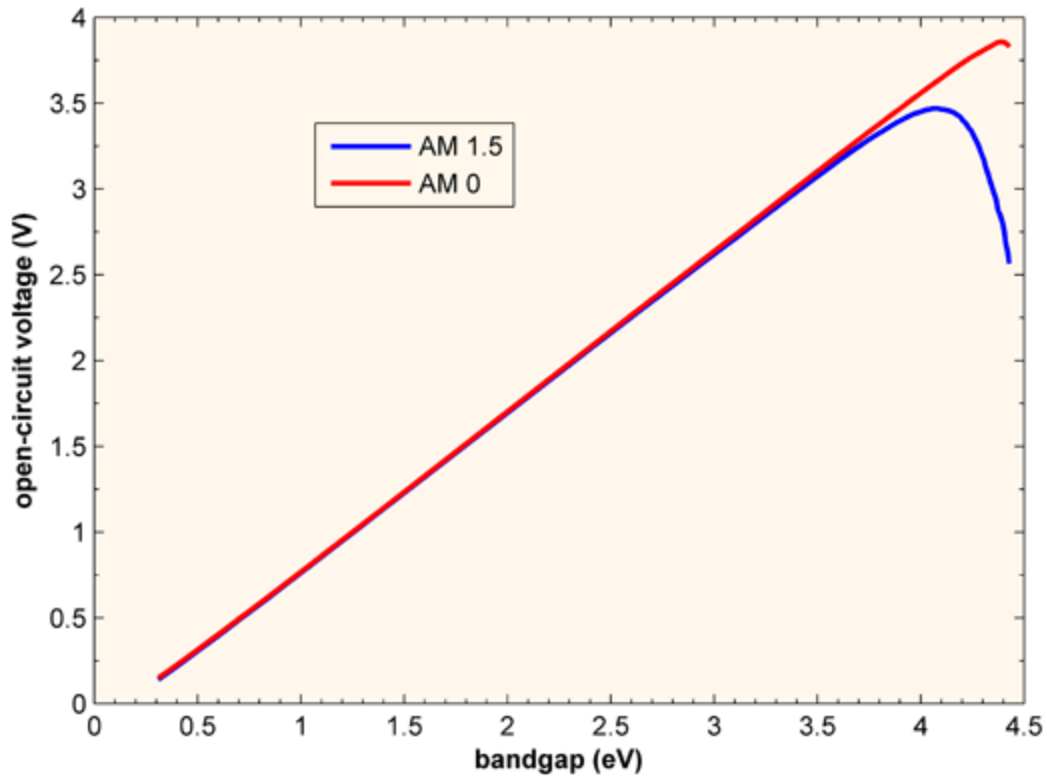
Fig 2.9: V_{OC} as function of band gap for a cell with AM 0 and AM 1.5. The V_{OC} increases with band gap as the recombination current falls. There is drop off in V_{OC} at very high band gaps due to the very low I_{SC}.

3. Fill Factor:

Another defining term in the overall behavior of a solar cell is the fill factor (FF). This is the available power at the maximum power point (P_m) divided by the open circuit voltage (V_{OC}) and the short circuit current (I_{SC}):

$$FF = \frac{V_{MP}I_{MP}}{V_{OC}I_{SC}}$$ .... (2.6)

The fill factor is directly affected by the values of the cell's series, shunt resistances and diodes losses. Increasing the shunt resistance (R_{sh}) and decreasing the series resistance (R_s) lead to a higher fill factor, thus resulting in greater efficiency, and bringing the cell's output power closer to its theoretical maximum.[12]

The Fill factor has a value around 80% for a normal silicon PV cell.
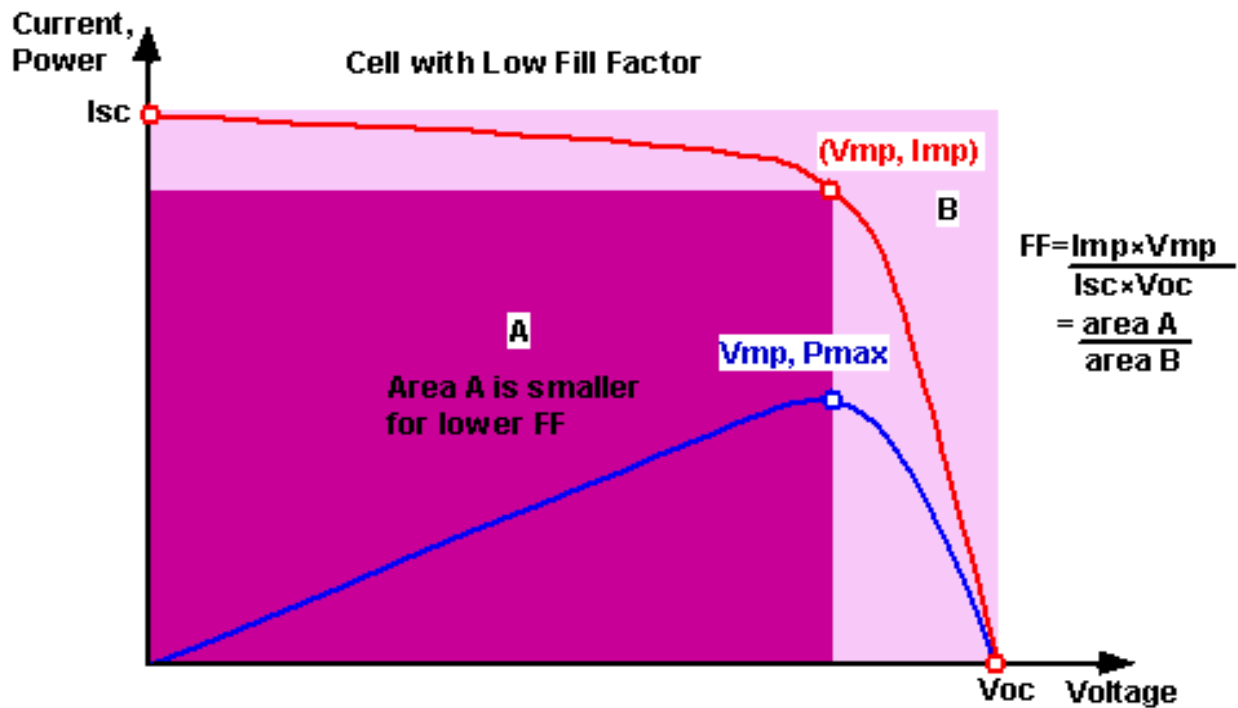
Fig 2.10: Graph of cell output current (red line) and power (blue line) as function of voltage

4. Efficiency:

The efficiency is the most commonly used parameter to compare the performance of one solar cell to another. Efficiency is defined as the ratio of energy output from the solar cell to input energy from the sun. In addition to reflecting the performance of the solar cell itself, the efficiency depends on the spectrum and intensity of the incident sunlight and the temperature of the solar cell. Therefore, conditions under which efficiency is measured must be carefully controlled in order to compare the performance of one device to another. Terrestrial solar cells are measured under AM1.5 conditions and at a temperature of 25°C. Solar cells intended for space use are measured under AM0 conditions.

The efficiency of a solar cell is determined as the fraction of incident power which is converted to electricity and is defined as:

$$P_{max} = V_{OC} I_{SC} FF$$

$$\eta = \frac{V_{OC} I_{SC} FF}{P_{in}}$$ ………………………………… (2.7)

Where Voc is the open circuit voltage

Isc is the short circuit current

FF is the fill factor

η is the Efficiency

The input power for efficiency calculations is 1 kW/m^2 or 100 mW/cm^2. Thus the input power for a 100 × 100 mm^2 cell is 10 W and for a 156 × 156 mm^2 cell is 24.3 W. [6789]

Chapter 3

Properties of semiconductors materials[10][11]

3.1 Indium arsenide:

Indium arsenide, InAs or indium monoarsenide, is a semiconductor composed of indium and arsenic. It has the appearance of grey cubic crystals with a melting point of 942 °C. It is a direct band gap material. InAs is well known for its high electron mobility and narrow energy band gap.

3.1.1 Basic Parameters at 300 K

Crystal structure   Zinc Blende

Group of symmetry T_d^2-F43m

Number of atoms in 1 cm^3 $3.59 \cdot 10^{22}$

de Broglie electron wavelength   400 A

Debye temperature   280 K

Density   5.68 g cm^{-3}

Dielectric constant (static)   15.15

Dielectric constant (high frequency)   12.3

Effective electron mass $0.023m_o$

Effective hole masses m_h $0.41m_o$

Effective hole masses m_{lp}	0.026m_o

Electron affinity	4.9 eV

Lattice constant	6.0583 A

Optical phonon energy	0.030 eV

3.1.2 Electrical properties

Breakdown field	$\approx 4 \cdot 10^4$ V cm^{-1}
Mobility of electrons	$\leq 4 \cdot 10^4$ cm^{2}V^{-1}s^{-1}
Mobility of holes	$\leq 5 \cdot 10^2$ cm^2 V^{-1}s^{-1}
Diffusion coefficient of electrons	$\leq 10^3$ cm^{2}s^{-1}
Diffusion coefficient of holes	≤ 13 cm^2 s^{-1}
Electron thermal velocity	$7.7 \cdot 10^5$ m s^{-1}
Hole thermal velocity	$2 \cdot 10^5$ m s^{-1}

3.1.3 Optical properties

Infrared refractive index	≈ 3.51 (300 K)

Radiative recombination coefficient	$1.1 \cdot 10^{-10}$ cm^3/s

3.1.4 Thermal properties

Bulk modulus	$5.8 \cdot 10^{11}$ dyn cm^{-2}

Melting point	942 °C

Specific heat	0.25 J g^{-1} °C^{-1}

Thermal conductivity   0.27 W cm^{-1} °C^{-1}

Thermal diffusivity   0.19 cm^{2}s^{-1}

3.2 Gallium arsenide:

Gallium arsenide (GaAs) is a compound of the elements gallium and arsenic. It is a III-V direct bandgap semiconductor with a zinc blende crystal structure. Gallium arsenide is used in the manufacture of devices such as microwave frequency integrated circuits, monolithic microwave integrated circuits, infrared light-emitting diodes, **laser diodes**, solar cells and **optical** windows.

3.2.1 Basic Parameters at 300 K

Crystal structure	Zinc Blende
Group of symmetry	T_d^2-F43m
Number of atoms in 1 cm^3	$4.42 \cdot 10^{22}$
de Broglie electron wavelength	240 A
Debye temperature	360 K
Density	5.32 g cm^{-3}
Dielectric constant (static)	12.9
Dielectric constant (high frequency)	10.89
Effective electron mass m_e	$0.063m_o$
Effective hole masses m_h	$0.51m_o$
Effective hole masses m_{lp}	$0.082m_o$
Electron affinity	4.07 eV
Lattice constant	5.65325 A
Optical phonon energy	0.035 eV

3.2.2 Electrical properties

Breakdown field	$\approx 4 \cdot 10^5$ V/cm
Mobility electrons	≤ 8500 cm^2 V^{-1}s^{-1}
Mobility holes	≤ 400 cm^2 V^{-1}s^{-1}
Diffusion coefficient electrons	≤ 200 cm^2/s
Diffusion coefficient holes	≤ 10 cm^2/s
Electron thermal velocity	$4.4 \cdot 10^5$ m/s
Hole thermal velocity	$1.8 \cdot 10^5$ m/s

3.2.3 Optical properties
Infrared refractive index 3.3

Radiative recombination coefficient $7 \cdot 10^{-10}$ cm^3/s

3.2.4 Thermal properties

Bulk modulus	$7.53 \cdot 10^{11}$ dyn cm^{-2}
Melting point	1240 °C
Specific heat	0.33 J g^{-1}°C^{-1}
Thermal conductivity	0.55 W cm^{-1} °C^{-1}
Thermal diffusivity	0.31 cm^{2}s^{-1}
Thermal expansion, linear	$5.73 \cdot 10^{-6}$ °C^{-1}

3.3 Indium antimonite:

Indium antimonite (InSb) is a crystalline semiconductor made of antimony and indium. It belongs to the III-V group and is a narrow gap semiconductor material. Detectors made of indium antimonite are sensitive and lie between a wavelength of 1 and 5 μm. Indium

antimonite was commonly used in mechanically scanned single detector thermal imaging systems.

3.3.1 Electrical Properties

The electrical properties of indium antimonite are provided in the table below:

Electrical Properties	
Intrinsic Carrier Concentration	$2x10^{16} cm^{-3}$
Electron Mobility	$\leq 7.7x10^{4} cm^2\ V^{-1}\ s^{-1}$
Hole Mobility	$\leq 850\ cm^2\ V^{-1}\ s^{-1}$
Electron Diffusion Coefficient	$\leq 2x10^{3}\ cm^2\ s^{-1}$
Hole Diffusion Coefficient	$\leq 22\ cm^2\ s^{-1}$
Electrical resistivity	$4x10^{-13} \Omega cm$

3.3.2 Thermal, Mechanical and Optical Properties

The thermal, mechanical and optical properties of indium antimonite are provided in the tables below:

Mechanical Properties	
Melting Point	527 °C
Density	$5.775\ g\ cm^{-3}$
Bulk Modulus	$4.7 \bullet 10^{11}\ dyn\ cm^{-2}$
Thermal Properties	
Thermal Conductivity	$0.18\ W\ cm^{-1}\ °C^{-1}$
Thermal Diffusivity	$0.16\ cm^2\ s^{-1}$

Thermal Expansion Coefficient	5.37×10^{-6} °C^{-1}

Optical Properties	
Refractive Index (589 nm @ 293 K)	4

3.3.3 Gallium antimonite:

Gallium antimonite (GaSb) is a semiconductor made of antimony and gallium belonging to the III to V semiconductor family. The lattice constant of GaSb is 0.61 nm. The unique lattice structure of GaSb enables its use in sophisticated semiconductor applications. For example, researchers at the Centre for Quantum Devices, Northwestern University, in January 2013 developed the first ever dual mode passive and active infrared camera chip made of gallium antimonite/indium arsenide.

3.3.4 Chemical Properties

The chemical properties of gallium antimonite are provided in the table below:

Chemical Properties	
Chemical Formula	GaSb
Molecular Weight	191.483 g/mol
CAS No.	12064-03-8
IUPAC Name	Gallium (III) antimonite
Group	III-V
Band Gap	0.726 eV
Band Gap Type	Indirect
Crystal Structure	Zinc Blende
Symmetry Group	T_d^2-F43m
Lattice Constant	6.09593 Angstroms

3.3.5 Electrical Properties

The electrical properties of gallium antimonite are provided in the table below:

Electrical Properties	
Intrinsic Carrier Concentration	$1.5 \times 10^{12} \text{cm}^{-3}$
Electron Mobility	$\leq 3000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$
Hole Mobility	$\leq 1000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$
Electron Diffusion Coefficient	$\leq 75 \text{ cm}^2 \text{ s}^{-1}$
Hole Diffusion Coefficient	$\leq 25 \text{ cm}^2 \text{ s}^{-1}$

3.3.6 Thermal, Mechanical and Optical Properties

The thermal, mechanical and optical properties of gallium antimonite are provided in the tables below:

Mechanical Properties	
Melting Point	712 °C
Density	5.614 g cm^{-3}
Bulk Modulus	$5.63 \cdot 10^{11} \text{ dyn cm}^{-2}$
Thermal Properties	
Thermal Conductivity	$0.32 \text{ W cm}^{-1} \text{ °C}^{-1}$
Thermal Diffusivity	$0.23 \text{ cm}^2 \text{ s}^{-1}$
Thermal Expansion Coefficient	$7.75 \times 10^{-6} \text{ °C}^{-1}$
Optical Properties	
Refractive Index (589 nm @ 293 K)	3,8
Radiative Recombination Coefficient (@ 300 K)	$10\text{-}10 \text{ cm}^3 \text{ s}^{-1}$

[33]

Chapter 4

Quantum well

A **quantum well** is a thin layer which can confine (quasi-)particles (typically electrons or holes) in the dimension perpendicular to the layer surface, whereas the movement in the other dimensions is not restricted. The confinement is a **quantum** effect.[12]
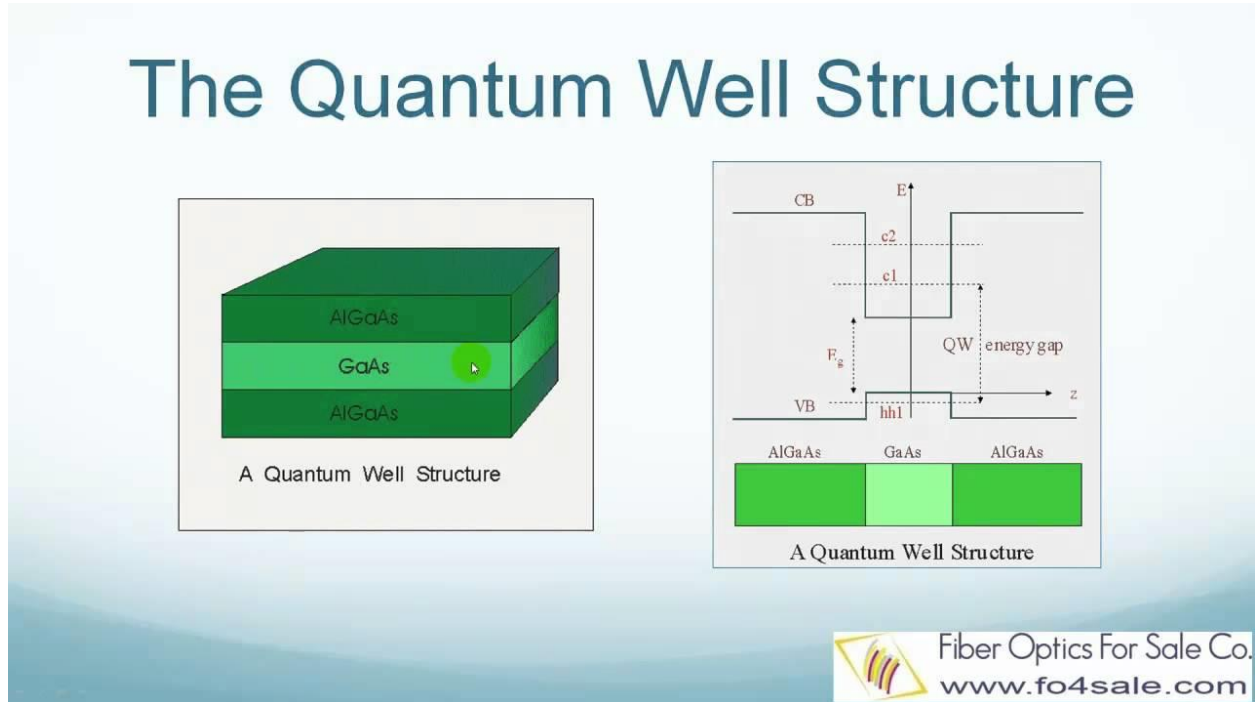

Fig 4.1: Structure of quantum well

4.1 Quantum well laser:

A **quantum well laser** is a laser diode in which the active region of the device is so narrow that quantum confinement occurs. Laser diodes are formed in compound semiconductor materials that (quite unlike silicon) are able to emit light efficiently. The wavelength of the light emitted by a quantum well laser is determined by the width of the active region rather than just the band gap of the material from which it is constructed.[1] This means that much longer wavelengths can be obtained from quantum well lasers than from conventional laser diodes using a particular semiconductor material. The efficiency of a quantum well laser is also greater than a conventional laser diode due to the stepwise form of its density of states function. [13]
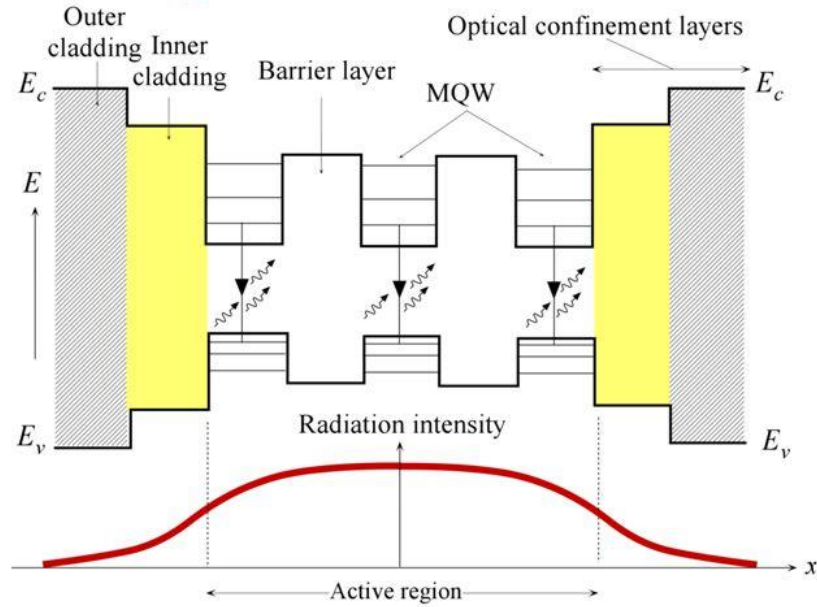
A simplified schematic diagram of multiple quantum well (MQW) heterostructure laser diode. Electrons are injected by the forward current into quantum wells. The light intensity distribution is also shown. Most of the light is in the active region.

Fig 4.2: Quantum well lasers.

4.2 Electrons and excitons in single QW potential:

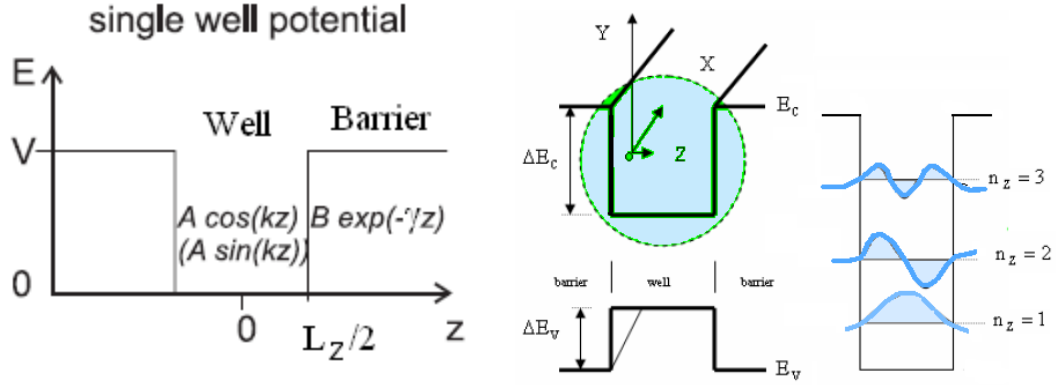The single QW is assumed as a square well potential of width □ and height V(z), as depicted in Fig.4.3.

Fig. 4.3 (a) Schematic picture of a single quantum well, (b) and energy levels.

The potential depth V(z) ($\Box E_c$ and $\Box E_v$) of semiconductor QW are known as band offset which are critical parameters in device simulation. Then the standard Schrodinger equation can be written for each of the semiconductor layers (QW and barrier layers) as follow:

$$\left[-\frac{\hbar^2}{2m_W^*}\frac{\partial^2}{\partial z^2}+V(z)\right]\psi(z)=E\,\psi(z),\quad z\leq-\frac{L_z}{2} \tag{4.1}$$

$$\left[-\frac{\hbar^2}{2m_{e,h}^*}\frac{\partial^2}{\partial z^2}\right]\psi(z)=E\,\psi(z),\quad \frac{L_z}{2}\leq z\leq\frac{L_z}{2} \tag{4.2}$$

$$\left[-\frac{\hbar^2}{2m_B^*}\frac{\partial^2}{\partial z^2}+V(z)\right]\psi(z)=E\,\psi(z),\quad z\geq-\frac{L_z}{2} \tag{4.3}$$

Where, m_W^* and m_B^* are the effective mass of the semiconductor layers act as QW and barriers.

The probability interpretation of the wave function requires that:

$$\int_z\psi^*(z)\psi(z)=1 \tag{4.4}$$

These further demand the condition:

$$\psi(z)\rightarrow 0,\text{ and }\frac{\partial}{\partial Z}\psi(z)\rightarrow 0, as\ z\rightarrow\pm\infty \tag{4.5}$$

Then the solutions for the even parity states would follow as:

[36]

$$
\psi(z) = \begin{cases} B\exp(\gamma z), & z \le \dfrac{L_z}{2} \\[2mm] A\cos(kz), & -\dfrac{L_z}{2} \le z \le \dfrac{L_z}{2} \\[2mm] B\exp(-\gamma z), & z \ge \dfrac{L_z}{2} \end{cases}
\tag{4.6}
$$

Using these trial forms of the wave function in their corresponding Schrödinger equation gives the constants:

$$
k = \frac{\sqrt{2m_W^* E}}{\hbar}, \quad \text{and} \quad \gamma = \frac{\sqrt{2m_B^*(V-E)}}{\hbar}
\tag{4.7}
$$

Now in order to proceed we need boundary conditions: both $\psi(z)$, $\dfrac{\partial}{\partial z}\psi(z)$ will be continuous and

at the interface of $z = +L_z/2$, the wave function and their derivatives in the well and barrier will be equal. These will lead to the following solution for even states:

$$
\tan\left(\frac{kL_z}{2}\right) = \frac{m_W^*\gamma}{m_B^*k}, \text{ or } \tan(kL_z) = \frac{2\dfrac{m_W^*\gamma}{m_B^*k}}{1-\dfrac{m_W^*\gamma}{m_B^*k}^2}
\tag{4.8}
$$

Similar derivation as above with sine-function replacing the *Acos(kz)* in equation (2.34) will give the odd states:

$$
\cot\left(\frac{kL_z}{2}\right) = \frac{m_W^*\gamma}{m_B^*k}
\tag{4.9}
$$

Such single value problems can be solved by both graphically and numerically. The solution for an even parity Eigen energies for InGaSb/AlGaSb is shown in Fig.2.8.

A certain penetration of the wave-function is also possible because the corresponding quantum mechanical particle would tunnel into or through the barrier of finite width b, and the transmission or tunnel probability can be derived as

$$
T(E) = e^{\frac{-4}{\hbar}b\sqrt{2m^*(V-E)}}
\tag{4.10}
$$

This means that the electronic tunnel-coupling of a particle with effective mass m* through a potential barrier of a fixed height, *V-E* decreases exponentially with the barrier width, i.e. the separation of two coupled QWs, dots, etc.

Despite the good achievement in the understanding of the electron properties in QW structures, for some type of experiment, it turned out to be favorable to not directly measure the electron properties, but to take advantage of the properties of electron-hole pairs, excitons. This is firstly because of the absence of coulomb interaction between the excitons and lattice since exciton have a total zero charge, and secondly the possibility to use their optical properties such as absorption of photon and their spontaneous radiative decay. These study include the work on time-integrated PL, time resolve PL, and absorption spectroscopy.

(a)

(b)

[38]
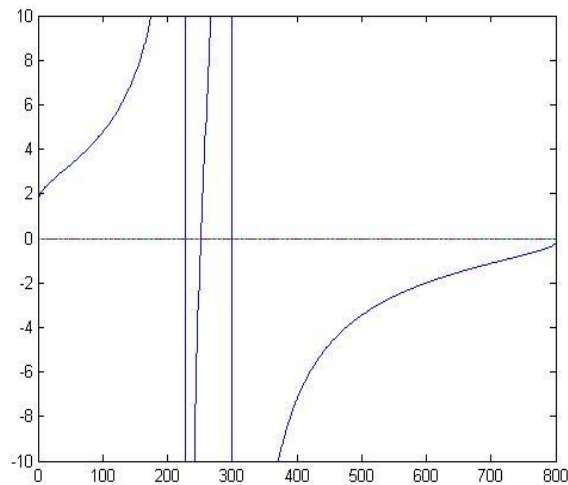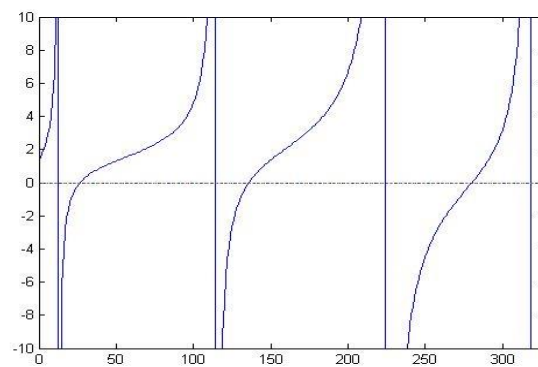
Fig.4.4 The solution for an even parity Eigen energies. (a) Eigen energies for conduction band confinements of InGaSb QW embedded in AlGaSb barrier for the QW height of L_z = 6 nm and (b) Eigen energies for valance band heavy-hole (hh) band confinements of InGaSb QW embedded in AlGaSb barrier for the QW height of Lz = 6 nm, where,

$$f(E) = \tan(kL_z) = 2\frac{m_W^* \gamma}{m_B^* k} \left/ 1 - \frac{m_W^* \gamma}{m_B^* k}^2 \right.$$

· ·

Chapter 5

Results and Discussion

5.1 Mat lab Code:

This is the mat lab code that uses for find the first confinement and second confinement of electron and hole. The mass of well and barrier are different for different materials. For this reason mass of well and barrier need to change for each material. Our main focus is to find different electron and hole confinement for different QW height(lz) of different materials.

Mw = 0.023; % mass of well

Mb = 0.067; % mass of barrier

h = 8.7292; % planks constant in mev

V = 800; % potential depth

Lz = 6; %QW height

e = zeros(1,1); % the dssired E values to be saved here

dif= zeros(1,1); % the difference between tan(klz) and the orher part)

k = zeros(1,1);

i =1;

j = 1;

l = 1;

for E= 1:1:V

   q = E;

   k = sqrt(Mw*q)/h;

   D = V-q;

gam = sqrt(2*Mb*D)/h;

```matlab
   y = tan(k*Lz);

   x = ((2*Mw*gam)/(Mb*k))/(1-(Mw*gam*gam)/(Mb*k));

   g = y - x;
dif(j) = g;        %saving the difference in diff

   j =j+1;          %increasing difs size

   G = abs(g);      % to measure how close the values are
if G < 0.0000001   % assuming equal if the difference is less than 0.0000001

e(i)= q;      % giving the corresponding E or q to the vector e

i= i+1;       % increasing i for next possible value

end

end

e% showing the values of determined E

F = 1:1:V;       % correspondig variable of E

plot(F,dif,F,x)         % plotting

axis ([0 V -10 10])    % axis shape

for F = 1:1:V

idF = find(abs(dif - x) == min(abs(dif - x)));

k(l) = F;

l = l+1;

end

xInter = F(idF);

disp(xInter);
```

We Have investigated four different configuration QW heterostructures including both binary and ternary semiconductors shown in Fig5.1 .

(a)
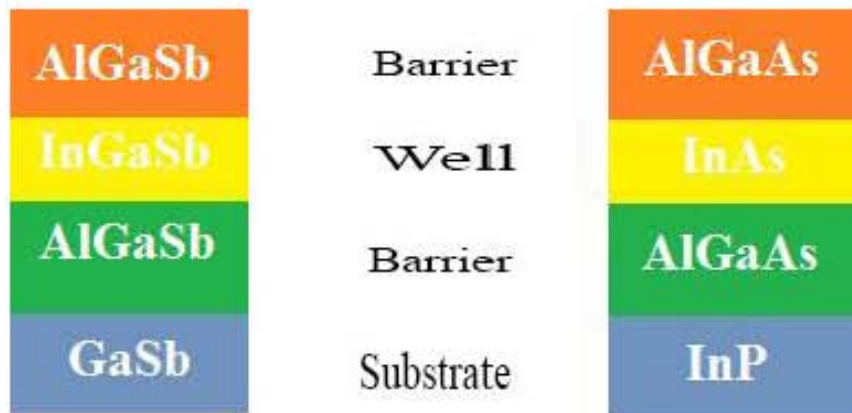
(b)

Fig 5.1: (a) Binary heterostructures (b) ternary heterostructures

5.2 Calculated Energy Band Structure:

We work with four different configurations. We can find energy band gap(Egw), potential depth(v) and band offset from energy band structure. Use this value we get the first confinement and second confinement. We assume 70% and 30% band offset.
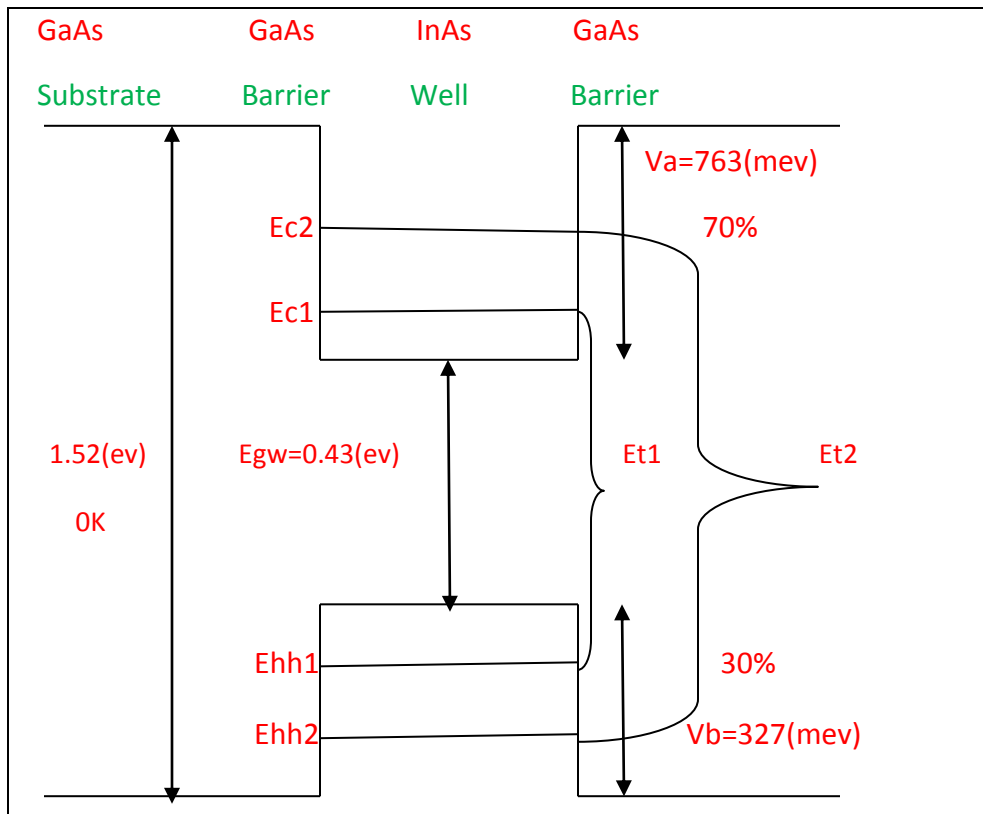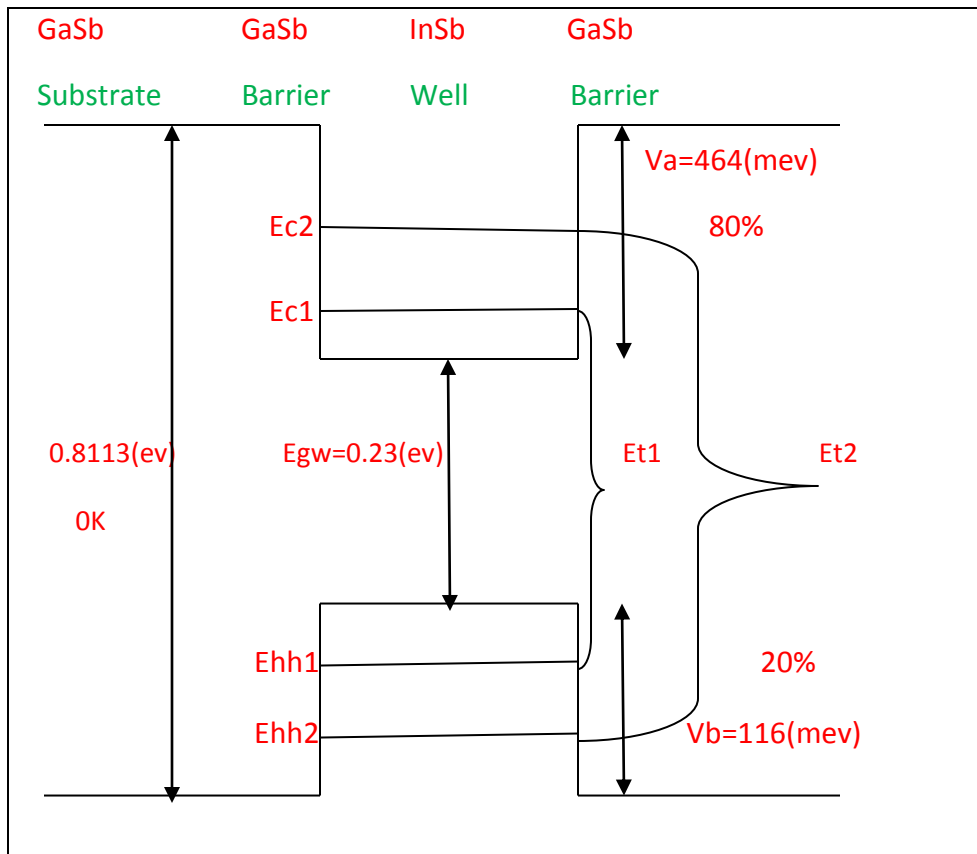

Fig 5.2 : Energy band Structure of InAs/GaAs QW
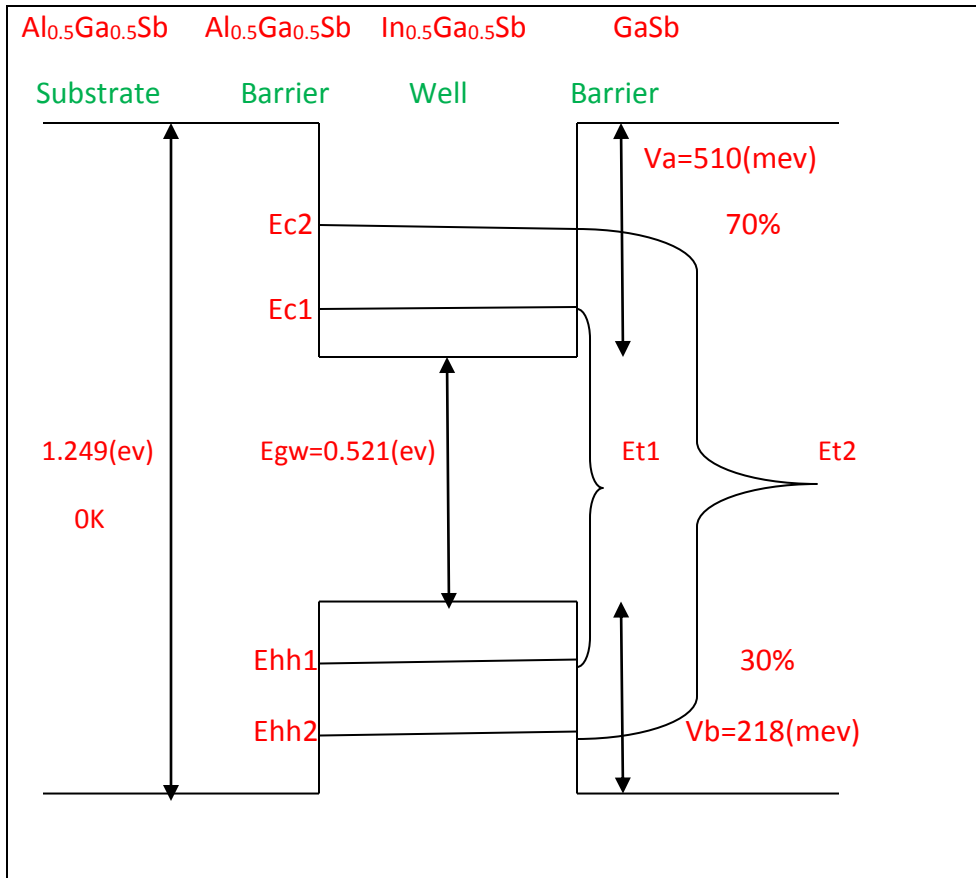
Fig 5.3: **Energy band Structure of GaSb/InSb QW**

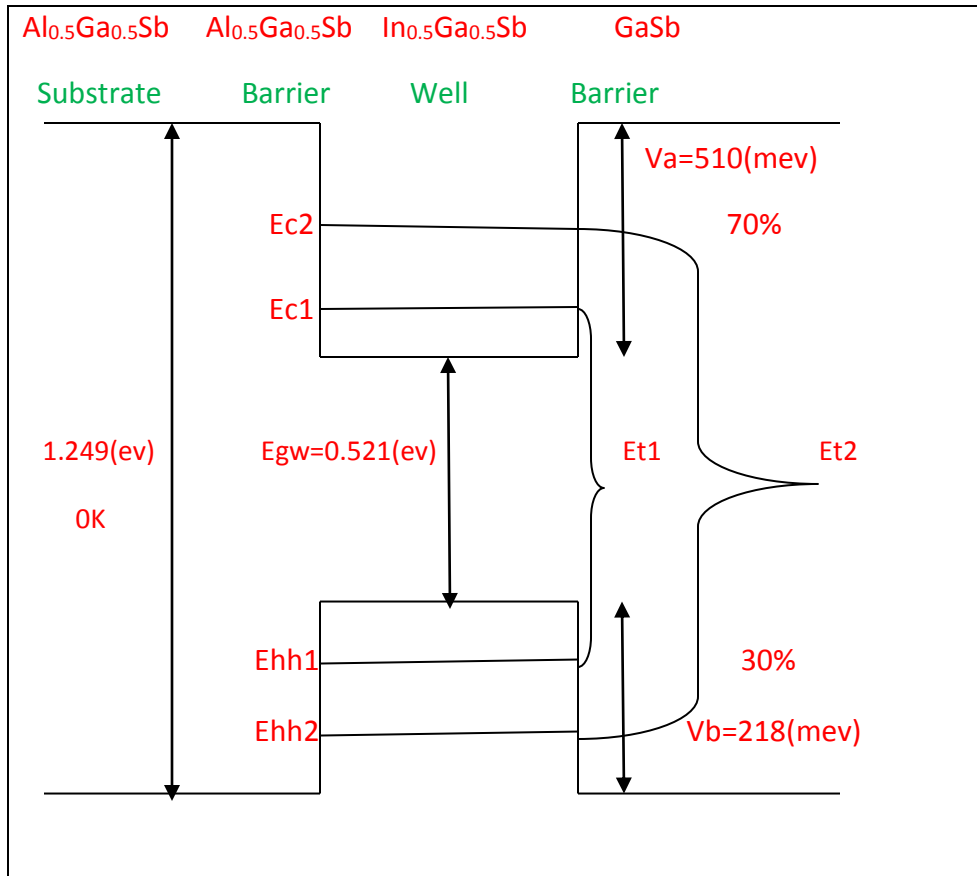**Fig 5.4: Energy band structure of AlGaSb/InGaSb**

Fig 5.5: Energy band Structure of AlGaSb/InGaSb

5.3 Confined level of Energies Listed in Table:

After getting the first and second confinement of electron and hole we generate a table. The table contain QW height (Lz), first electron confinement (Ec1), Second electron confinement (Ec2), first hole confinement (Eh1), Second electron confinement (Eh2). After that we calculate first confinement (Et1) and second confinement (Et2). We can find the exciting state from the table and corresponding graph.

Table 1:

Electron and Hole Confinement of InAs/GaAs

Lz	Ec1	Ec2	Ehh1	Ehh2	Egw	Et1=(Ec1+Eh1+ Egw)	Et2=(Ec2+Eh2 +Egw)
0.5	748		309		430	1487	
1	708		269		430	1407	
1.5	655		217		430	1302	
2	598		164		430	1192	
2.5	541		122		430	1093	
3	486		92		430	1008	
3.5	434		71		430	935	
4	387		56		430	873	
4.5	345		45		430	820	
5	307		37		430	774	
5.5	274		31		430	735	
6	245		27		430	702	
6.5	220	763	23	118	430	673	1311
7	198	753	20	103	430	648	1286
7.5	179	727	17	91	430	626	1248
8	162	694	15	81	430	607	1205
8.5	147	660	14	72	430	591	1162

Here, when Lz = 6.5 we get exiting states.
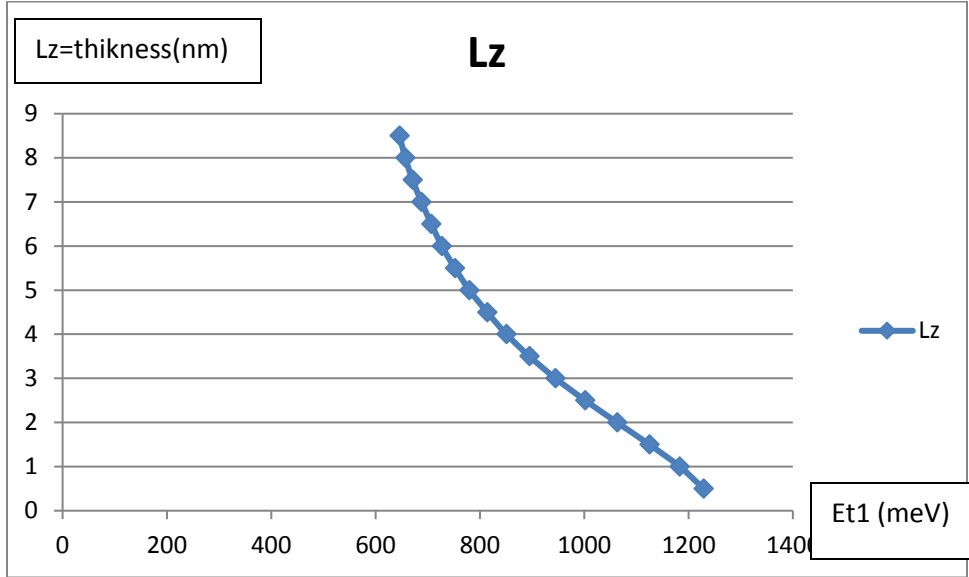
Fig1(a): First confinement of InAs/GaAs
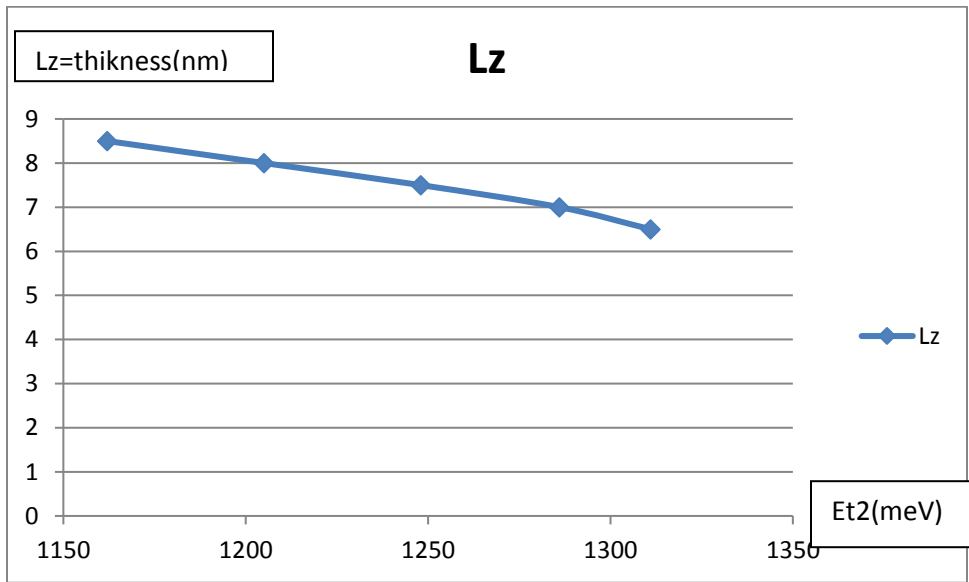
Fig1(b): Second Confinement of InAs/GsAs

[48]

Table 2:

Electron and Hole Confinement of GaSb/InSb

Lz	Ec1	Ehh1	Egw	Et1
0.5	460	114	230mev/0.23ev	804
1	450	107	230	787
1.5	434	96	230	760
2	413	82	230	725
2.5	390	68	230	688
3	366	56	230	652
3.5	341	46	230	617
4	316	38	230	584
4.5	293	32	230	555
5	270	27	230	527
5.5	249	23	230	502
6	230	19	230	479
6.5	212	17	230	459
7	195	15	230	440
7.5	180	13	230	423
8	167	11	230	408
8.5	154	10	230	394

Here, There is no exiting states exits

Fig 1: First confinement of GaSb/InSb

Table 3:

Electron and Hole Confinement of AlGaSb/ InGaSb

Lz	Ec1	Ec2	Ehh1	Ehh2	Egw	Et1=(Ec1+Eh1+Egw)	Et2=(Ec2+Eh2+Egw
0.5	502		206		521	1229	
1	479		183		521	1183	
1.5	448		156		521	1125	
2	413		129		521	1063	
2.5	377		104		521	1002	
3	342		82		521	945	
3.5	308		66		521	895	
4	277		53		521	851	
4.5	249		44		521	814	
5	223		36		521	780	
5.5	200		31		521	752	
6	180		26		521`	727	
6.5	163		23		521	707	
7	147	510	20	98	521	688	1129
7.5	133	508	17	88	521	671	1117
8	121	496	15	78	521	657	1095
8.5	111	479	14	71	521	646	1071

Here, when Lz = 7 then we get exiting states.
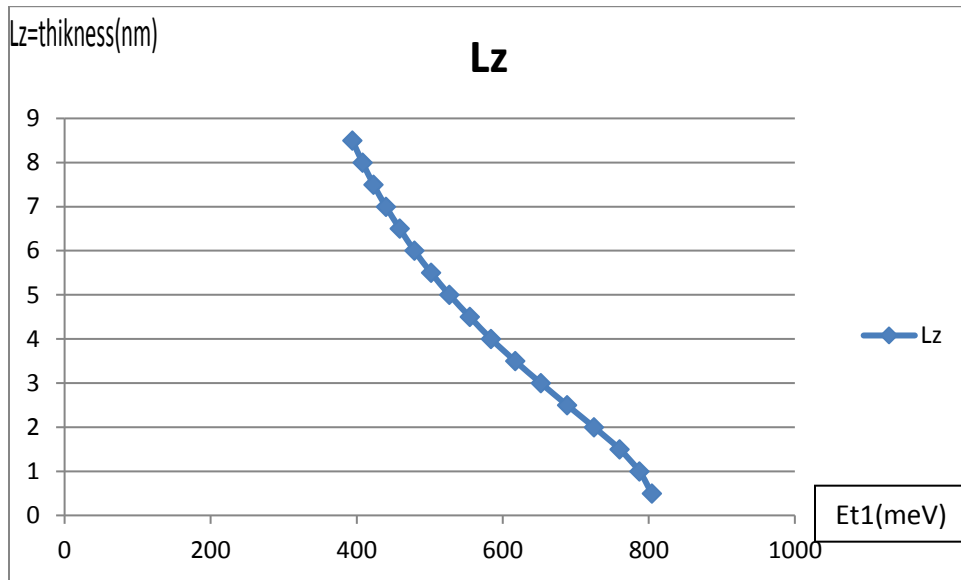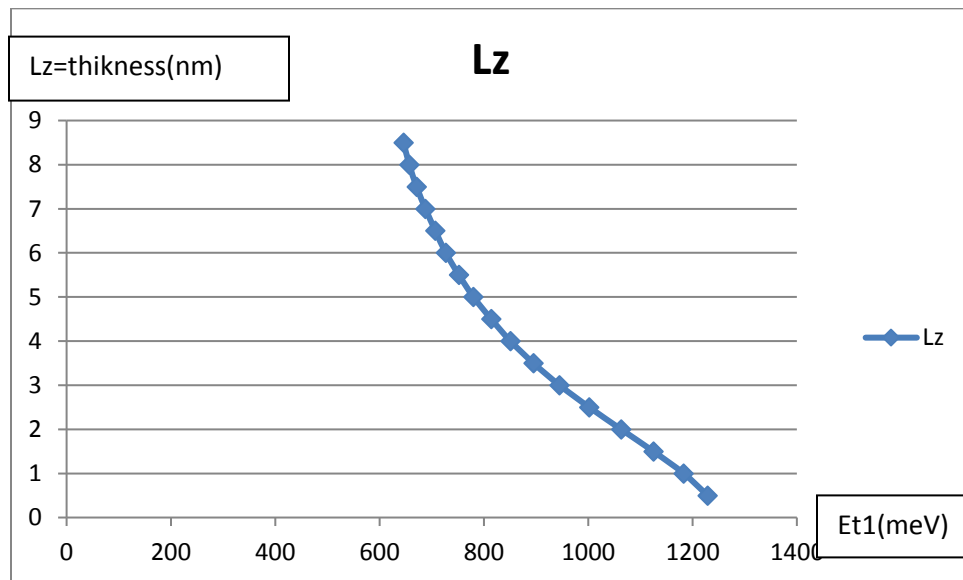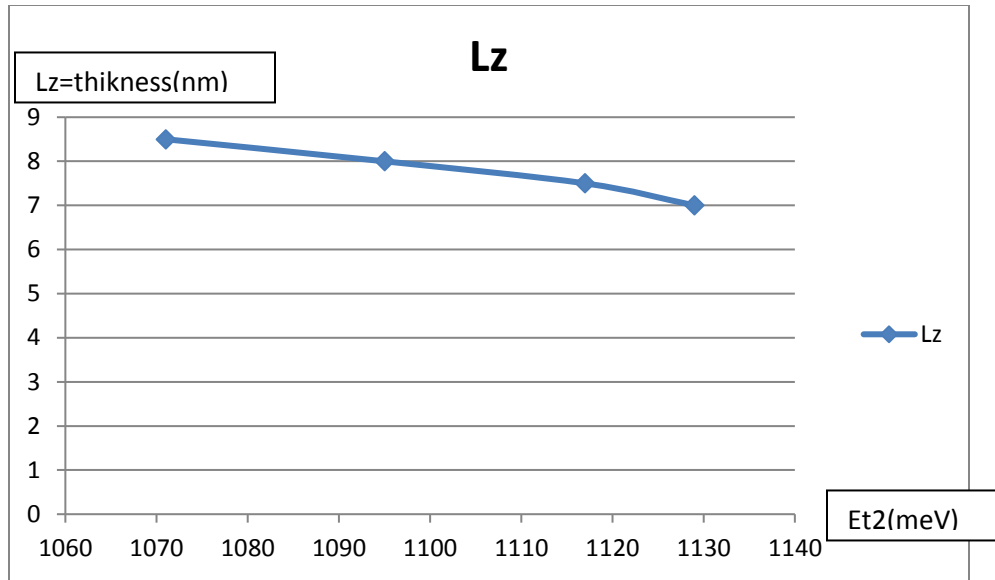

Fig 1(a): First confinement of AlGaSb/ InGaSb

Fig 1(b): Second Confinement of AlGaSb/ InGaSb

Table 4:

Electron and Hole Confinement of AlGaAs/InAs :

| Lz	Ec1	Ec2	Ehh1	Ehh2	Egw	Et1	Et2
0.5	974		401		430	1805	
1	889		342		430	1661	
1.5	801		272		430	1503	
2	719		202		430	1351	
2.5	645		146		430	1221`	
3	578		109		430	1117	
3.5	518		83		430	1031	
4	463		65		430	958	
4.5	413		52		430	895	
5	369		43		430	842	
5.5	330		36		430	796	
6	295	1001	30	148	430	755	1579
6.5	265	952	26	128	430	721	1510
7	239	896	23	112	430	692	1438
7.5	216	841	20	97	430	666	1368
8	196	790	17	87	430	643	1307
8.5	178	741	16	78	430	624	1249

Here, when Lz = 6 then we get exiting states.
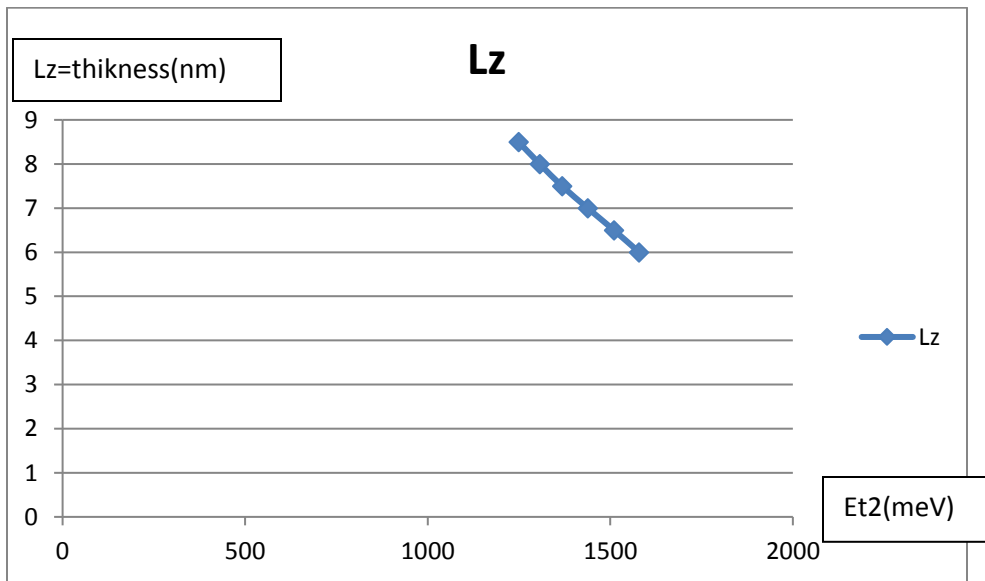
[51]
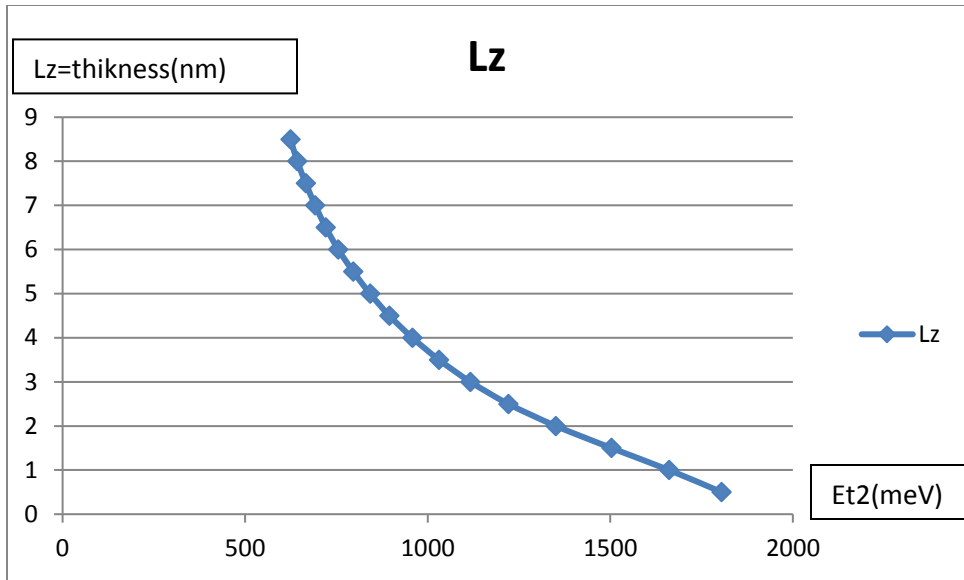
Fig 1(a): First confinement of AlGaAs/InAs

Fig 1(b): Second Confinement of AlGaAs/InAs

Chapter 6

6.1 Comparison the results with solar cell spectrum:

The spectrum of solar light at the Earth's surface is mostly spread across the visible and infrared (IR) ranges with a small part in the near-ultraviolet range. The visible and near-ultraviolet components of solar light are converted to the electricity and IR only heats solar cells. This heating has two negative reasons- firstly this heating can break the solar cell. This is because cells are produced from semiconductors that don't like to be heated. The second reason is the pointless losses of solar energy – instead of being converted to electricity, the energy is lost to heat. IR makes a significant contribution to the solar spectrum – it is approximately half of all solar energy, and so it is important to filter it out.

Solar radiation spectrum:
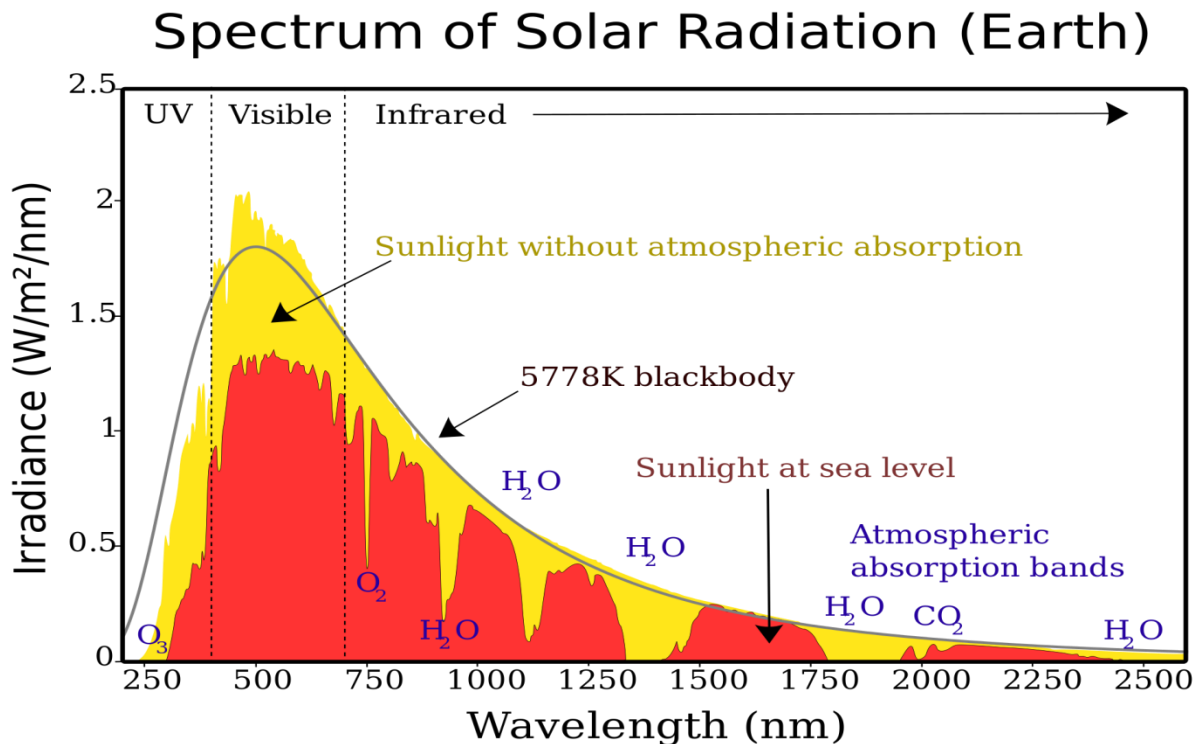
Spectrum of Solar Radiation (Earth)

Fig 6.1: Solar irradiance spectrum above atmosphere and at surface. Extreme UV and X-rays are produced (at left of wavelength range shown) but comprise very small amounts of the Sun's total output power.

6.2 Analyses of Quantum dot solar cell spectrum

Quantum dot solar cell can capture the entire solar spectrum but in this section we discussed about 4 types of even parity Eigen energies which also capture solar radiation spectrum as shown in Figure 6.1.

6.2.1 Convert energy gap to wavelength λ :

We know, the photon energy E and wavelength λ related as:

$$E(eV) = h\upsilon = \frac{hc}{\lambda} = \frac{1240}{\lambda(nm)}$$

$$\lambda\ (nm) = \frac{1240}{E(ev)} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(6.1)$$

Here we compare our finding with solar spectrum. Solar spectrum is efficient from 250(nm) to 2500(nm) range. We convert first confinement energy (eV) to wave length (nm). That shows in tables. The corresponding graph show the comparison with solar spectrum.

Table 5:

Convert the Energy Confinement states of GaAs/InAs with respect to λ

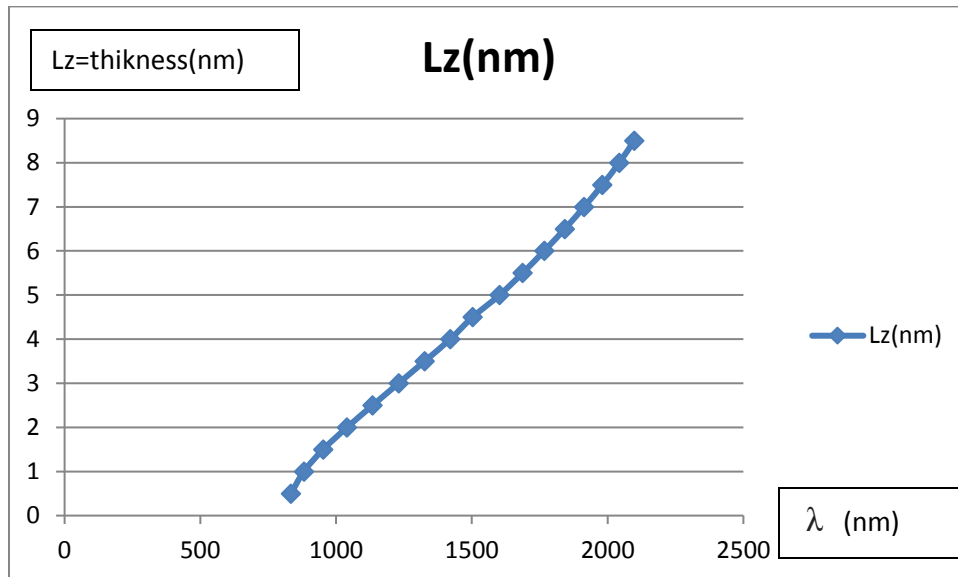| Et1(eV)	λ (nm)	Lz	Et2(eV)	λ (nm)
1.487	833.9	0.5		
1.407	881.3	1		
1.302	952.4	1.5		
1.192	1040.3	2		
1.093	1134.5	2.5		
1.008	1230.2	3		
0.935	1326.2	3.5		
0.873	1420.4	4		
0.825	1503.0	4.5		
0.774	1602.1	5		
0.735	1687.1	5.5		
0.702	1766.4	6		
0.673	1842.5	6.5	1.311	945.8
0.648	1913.6	7	1.286	964.2
0.626	1980.8	7.5	1.248	993.6
0.607	2042.8	8	1.205	1029.0
0.591	2098.1	8.5	1.162	1067.1

Fig 1(a): Wavelength λ vs Lz graph for first confinement energy states of GaAs/InAs which covered the wavelength of solar spectrum from 833 to 2098(nm).
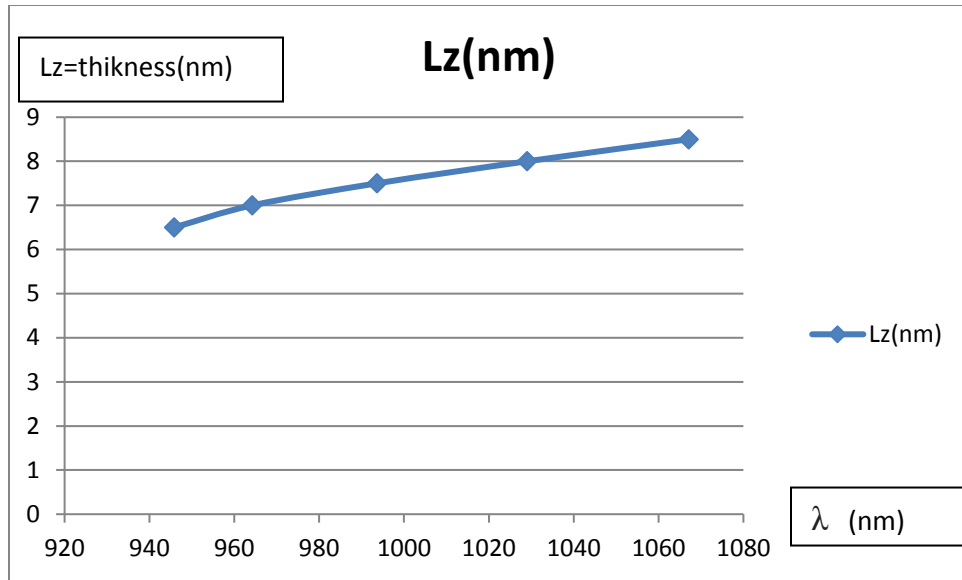
Fig 1(b): Wavelength λ vs Lz graph for secound confinement energy states of GaAs/InAs which covered the wavelength of solar spectrum from 945 to 1067(nm).

Table 6:

Convert the Energy Confinement states of GaSb/InSb with respect to λ

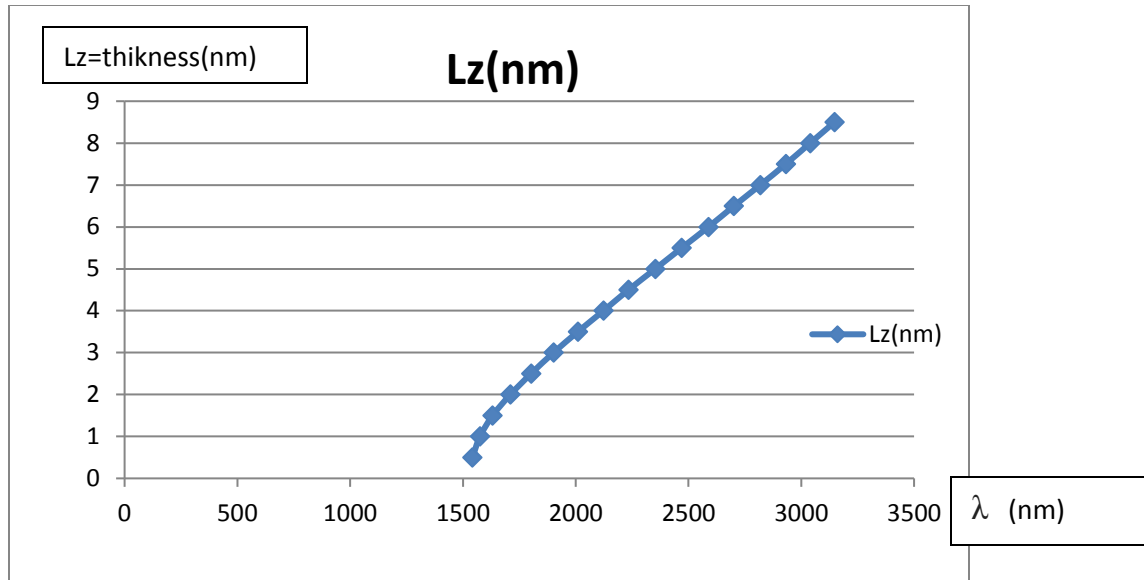| Et1(ev)	λ (nm)	Lz
0.804	1542.3	0.5
0.787	1575.6	1
0.760	1631.6	1.5
0.725	1710.3	2
0.688	1802.3	2.5
0.652	1901.8	3
0.617	2009.7	3.5
0.584	2123.3	4
0.555	2234.2	4.5
0.527	2352.9	5
0.502	2470.1	5.5
0.479	2588.7	6
0.459	2701.5	6.5
0.440	2818.1	7
0.423	2931.4	7.5
0.408	3039.2	8
0.394	3147.2	8.5

Fig 1: Wavelength λ vs Lz graph for first confinement energy states of GaSb/InSb which covered the wavelength of solar spectrum from 1542 to 3147(nm).

Table7:

Convert the Energy Confinement states of AlGaSb/InGaSb with respect to λ

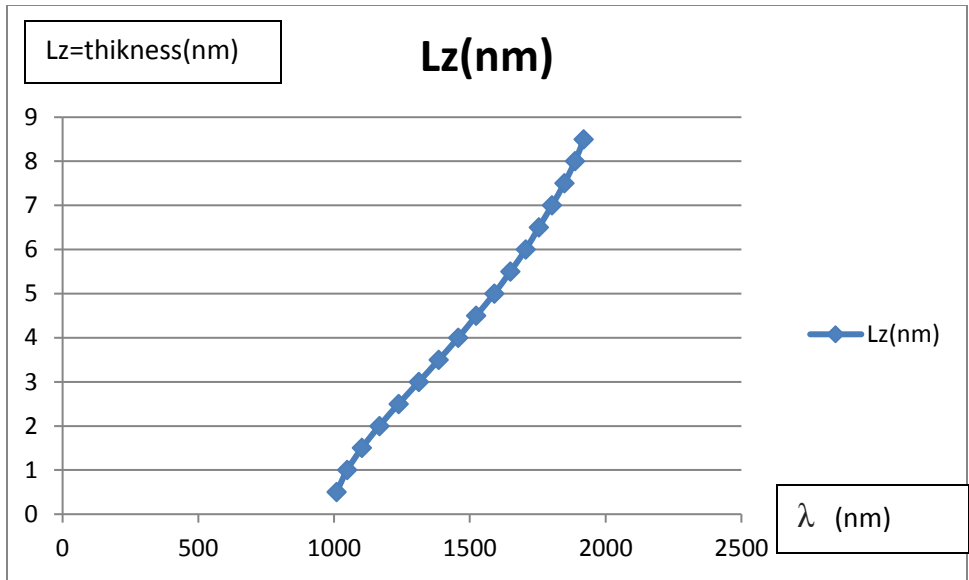| Et1(ev)	λ (nm)	Lz(nm)	Et2(ev)	λ (nm)
1.229	1008.9	0.5		
1.183	1048.2	1		
1.125	1102.2	1.5		
1.063	1166.5	2		
1.002	1237.5	2.5		
0.945	1312.2	3		
0.895	1385.5	3.5		
0.851	1457.1	4		
0.814	1523.3	4.5		
0.780	1589.7	5		
0.752	1648.9	5.5		
0.727	1705.6	6		
0.707	1753.9	6.5		
0.688	1802.3	7	1.129	1098.3
0.671	1847.9	7.5	1.117	1110.1
0.657	1887.3	8	1.095	1132.4
0.646	1919.5	8.5	1.071	1157.8

Fig 1(a): Wavelength λ vs Lz graph for first confinement energy states of AlGaSb/InGaSb which covered the wavelength of solar spectrum from 1008 to 1919(nm).
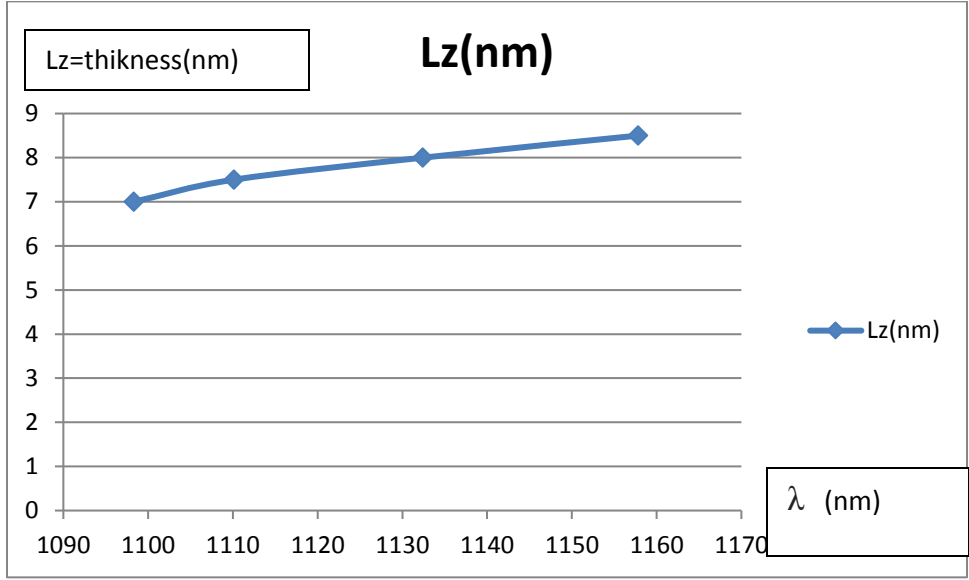

Fig 1(b): Wavelength λ vs Lz graph for secound confinement energy states of AlGaSb/InGaSb which covered the wavelength of solar spectrum from 1098 to 1158(nm).

Table 8:

Convert the Energy Confinement states of AlGaAs/InAs with respect to λ

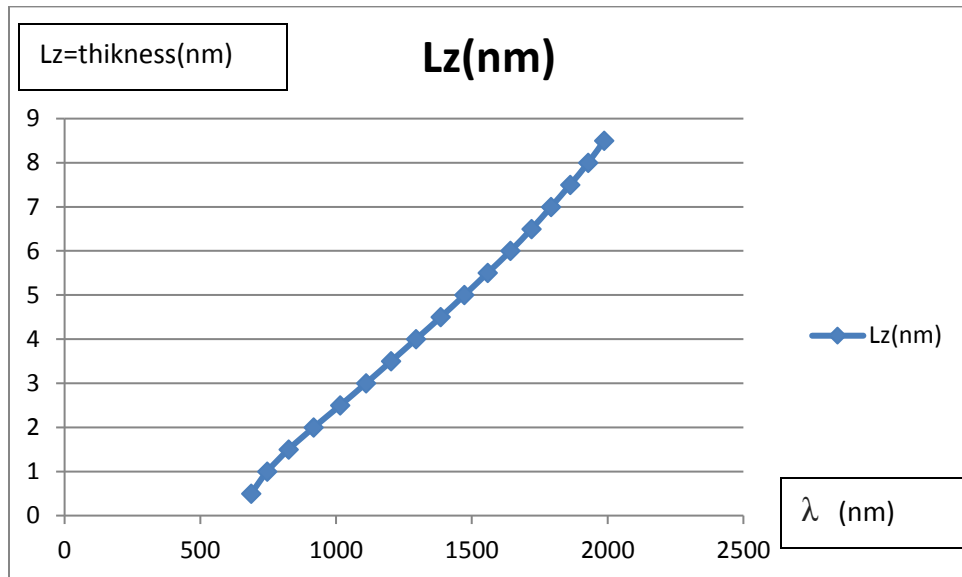| Et1(ev)	λ (nm)	Lz(nm)	Et2(ev)	λ (nm)
1.805	687.0	0.5		
1.661	746.5	1		
1.503	825.0	1.5		
1.351	917.8	2		
1.221	1015.6	2.5		
1.117	1110.1	3		
1.031	1202.7	3.5		
0.958	1294.3	4		
0.895	1385.5	4.5		
0.842	1472.7	5		
0.796	1557.8	5.5		
0.755	1642.4	6	1.579	785.3
0.721	1719.8	6.5	1.510	821.2
0.692	1791.9	7	1.438	862.3
0.666	1861.9	7.5	1.368	906.4
0.643	1928.5	8	1.307	948.7
0.624	1987.2	8.5	1.249	992.8

Fig 1(a): Wavelength λ vs Lz graph for first confinement energy states of AlGaAs/InAs which covered the wavelength of solar spectrum from 687 to 1987(nm).
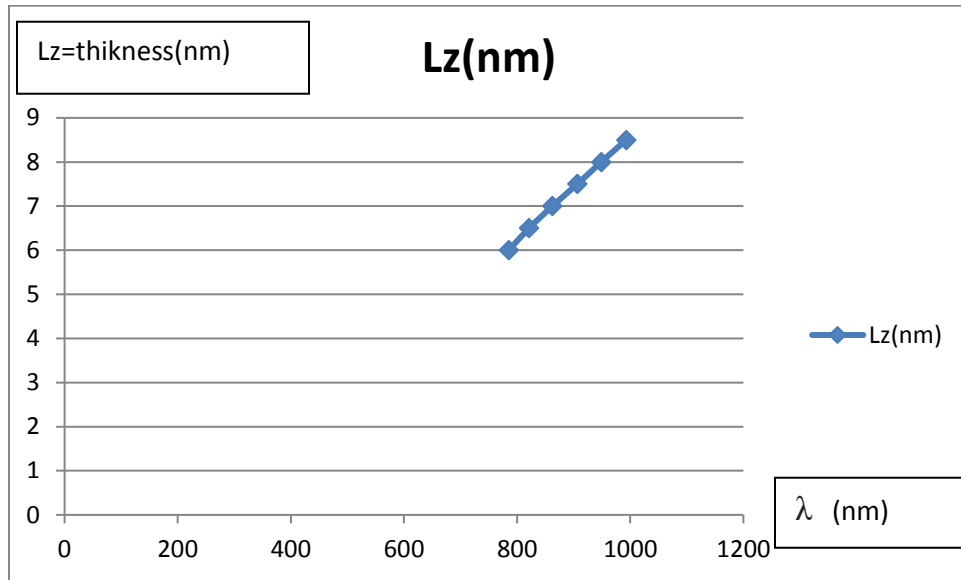
Fig 1(b): Wavelength λ vs Lz graph for secound confinement energy states of AlGaAs/InAs which covered the wavelength of solar spectrum from 785 to 993(nm).

Chapter 7

Conclusion and Future work

7.1 Conclusion:

In this work we have theoretically investigated the confined energy states of excitons in low dimensional quantum-well heterostructures. The objective of the work lies on the capturing of as many photons as possible from the whole range of solar radiation by the quantum well-based solar cell structures. Therefore, different sets of sample hetero-structures have been used to demonstrate the importance of our investigation. Since it is known that a thermal-activated behavior of the excitons in the quantum well is one of the key issues limiting the open circuit voltage and thus the efficiency of a solar cell, therefore we have also calculated the excited states of excitons in all these structures. The calculation is performed by solving Schrödinger equation for finite potential well. For InAs/GaAs QW-structure the conduction band offset was chosen 70% while for InSb/GaAb about 90%. Our results have shown that 1st confined energy states of InAs/GaAs QW cover the energy range of 591 to 1487(meV), the 2nd confined energy range of 1162 to 1311(meV). Semilarly for InSb/GaSb cover the energy range of 394 to 804. For AlGaSb/InGaSb 1st confined energy range of 646 to 1229(mev), the 2nd confined energy range of 1071 to 1129(meV) and for AlGaAs/InAs 1st confined energy range of 624 to 1805(meV) , the 2nd confined energy range of 1249 to 1579(meV). We believe that our investigation will contribute understating and designing the QW/dot-based solar cell structures in near future.

7.2 Future work:

 Analysis of temperature dependent energy band gap of quantum well/dot using varshni relation.

References:

1. http://whatis.techtarget.com/definition/semiconductor
2. Properties of Semiconductor https://en.wikipedia.org/wiki/Semiconductor
3. Photovoltic Generation http://www.plasticphotovoltaics.org/lc/lc-solarcells/lc-introduction.
4. https://en.wikipedia.org/wiki/List_of_types_of_solar_cells
5. Amorphous Silicon solar cell https://en.wikipedia.org/wiki/Amorphous_silicon
6. Volker Quaschning, Regenerative Energiesysteme. Technologie – Berechnung – Simulation. 8th. Edition. Hanser (Munich) 2013, p. 49.
7. "Publications, Presentations, and News Database: Cadmium Telluride". National Renewable Energy Laboratory.
8. K. Zweibel, J. Mason, V. Fthenakis, "A Solar Grand Plan", *Scientific American*, Jan 2008. CdTe PV is the cheapest example of PV technologies and prices are about 16¢/kWh with US Southwest sunlight.
9. Further mention of cost competitiveness: "Solar Power Lightens Up with Thin-Film Technology", Scientific American, April 2008
10. http://www.ioffe.ru/SVA/NSM/Semicond/InAs/GaAs
11. http://www.azom.com/article.aspx?ArticleID=8356
12. https://www.rp-photonics.com/**quantum_wells**.html]
13. https://en.wikipedia.org/wiki/Quantum_well_laser