SIMULATION AND THEORETICAL ANALYSIS OF QUANTUM DOT SOLAR CELLS

A dissertation report

submitted in the partial fulfillment of the requirements for the award of the degree

of

MASTER OF TECHNOLOGY

in

ELECTRONICS & COMMUNICATION

(With specialization in Micro Electronic and VLSI)

Submitted by

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May 2016

CANDIDATE'S DECLARATION

I hereby declare that the work which is being presented by me in this dissertation report entitle **"SIMULATION AND THEORETICAL ANALYSIS OF QUANTUM DOT SOLAR CELLS"** submitted in partial fulfillment of the requirement for the award of the degree of, **"Master of Technology in Electronics & Communication Engineering"** with specialization in **"Micro Electronic and VLSI"**, and submitted to the Department of Electronics & Communication Engineering, Indian Institute of Technology, Roorkee, is an authentic record of the work carried out by me during the period June 2015 to November 2015, under the guidance of **Dr. Brijesh Kumar,** Assistant Professor, Electronics & Communication Engineering Department, Indian institute of Technology, Roorkee.

Date:

Place: IIT, Roorkee **(KARAN SINGH)**

Enrollment No.-14534007

CERTIFICATE

This is to certify that the above statement made by the candidate is correct to the best of my knowledge.

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(KARAN SINGH)

Enrollment No.-14345007

M.Tech (Microelectronics &VLSI)

ABSTRACT

Solar cell works on the principle of photovoltaic which converts solar energy to electric energy. This thesis is based on simulation and theoretical analysis of quantum dot solar cells having Gallium Arsenide (GaAs) direct band gap material instead of conventional silicon which is indirect gap material and self-assembled Indium Arsenide (InAs) quantum dots (QDs) embedded inside the middle part of intrinsic layer of p-i-n structured solar cell which improves overall efficiency of solar cells up to 24.72% because limitations of conventional single junction solar cell is that it does not absorbs low energy photons to generate electron hole pairs thus these photons is not contributing in the device current and photons having high energy is not used efficiently as high energy photon generates hot carriers. In this work we proposed quantum dot (QD) intermediate band solar cell which absorbs photons having low energy in infrared region and contribute in the device current which increases external quantum efficiency of solar cell while maintaining open circuit voltage almost constant. We also increased intrinsic layer in the structure and found that only increasing intrinsic layer short circuit current of device increases while open circuit voltage increases negligibly. Size of quantum dots, spacing between adjacent quantum dots and barrier material that separate two layers of quantum dot is challenging task, we used 5*10nm size of InAs, barrier material layer which is intrinsic GaAs of thickness 12.5nm and space between two adjacent filled with intrinsic GaAs is of 10nm width. Position of these quantum dots in intrinsic layer plays important role to increase external quantum efficiency (EQEs), we have placed these layers at middle of intrinsic layer. For all these simulation we used Silvaco Atlas TCAD software and got plots on Tony Plot.

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ABBEREVIATIONS

QDs……..Quantum Dots

QDSCs……Quantum Dot Solar Cells

InAs…….....Indium Arsenide

GaAs ……Gallium Arsenide

InGaP ……...Indium Gallium Phosphor

p…….....Holes concentration in p-type semiconductor

n …… ..Electrons concentration in n-type semiconductor

$\mathbf{J_{SC}}$……..Short circuit current

$\mathbf{V_{OC}}$……....Open circuit current

$\mathbf{U_{n0}}$……Electron mobility

$\mathbf{U_{p0}}$……Hole mobility

ni…….intrinsic concentration

si…….Wave function

$\mathbf{t_n}$…….Electron lifetime

$\mathbf{t_p}$…….Hole lifetime

TMUN……...Lattice temp. coefficient for electron mobility

TMUP….....Lattice temp. coefficient for of hole mobility

MUN…….Electron mobility

MUP…….Hole mobility

Umax.n…….....Mobility's of majority carriers

Umin.n…….....Mobility's of minority carrie

1. INTRODUCTION

1.1 Solar Energy

In modern time energy is essential for economic development of any country and fossil fuels is the main source around 85% of the total consumption of energy worldwide but due to limitations and shortage of fossil fuels there is energy crisis over the world, so there is best way to utilize green energy that is wind energy, solar energy, hydroelectric energy, geothermal energy, nuclear energy, tidal energy among these energies hydroelectric and tidal energy are limited by geography of earth and nuclear energy is used only in developed countries of the world because it requires sophisticated technology and money so solar energy is only which is available everywhere on earth which can be convert into electrical energy easily without harming nature as it does not create pollution and safer to use. The Sun which is 4.6 billion year old star only a source of solar energy, with mass $2*10^{30}$Kg and radius of 700,000Km. The surface temperature of sun is estimated as 6000^{o}K and core temperature $14*10^{6o}$ K due to such a high temperature nuclear fusion reaction takes place. Energy that is arriving outside the earth's atmosphere is 1365W/m^2 at spectral distribution of solar energy called (AM0) air mass zero. As it approaches to surface of the earth, due to infrared absorption it is attenuated. As photons passes though the atmosphere of earth, photons either scatter off water vapors, smoke, dust and various particles, are absorbed by certain components of atmosphere or reflected by clouds. A portion of the scattered radiation reaches the earth's surface and the rest diffuses into space. It emits electromagnetic radiation in visible, infrared, ultraviolet, x and y ray spectra. The configuration of emitted spectrum by sun is well defined by radiation of black body temperature about 5800^{o} K. The energy of the electromagnetic spectrum distribution at each wavelength in the useful range of the spectrum is illustrated in Figure 1.1

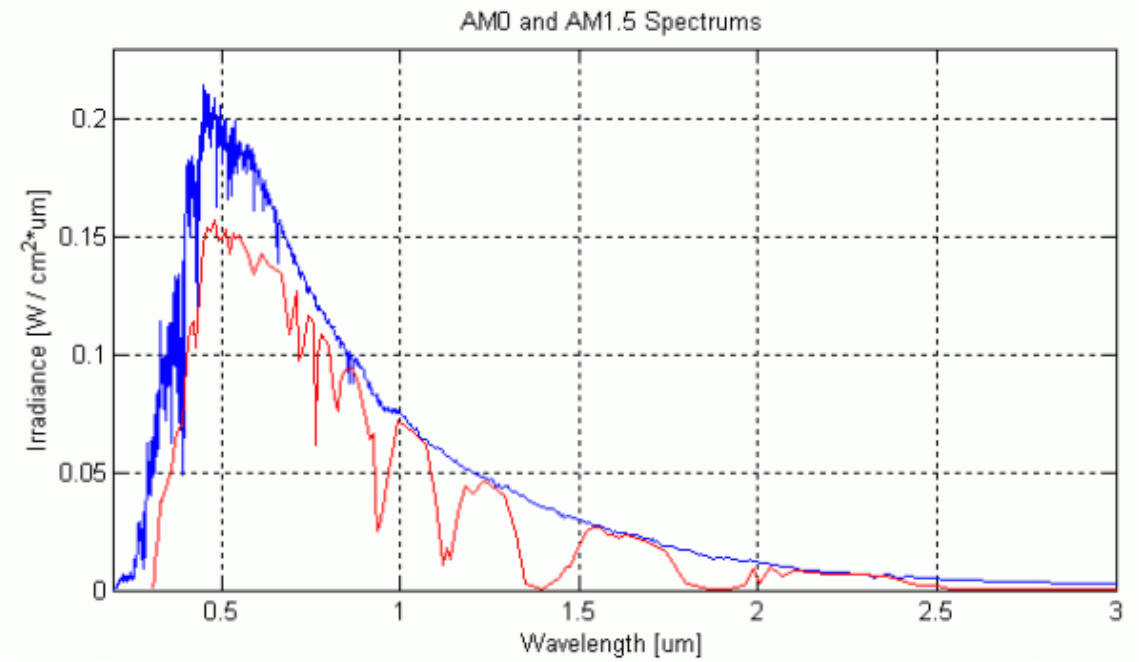


Fig.1.1 Solar energy spectral distributions when AM1.5 (red) and AM1 (blue) (data after Ref. [1])

Most of the power of sun light is in visible spectra.

Height	**Sun's position**	**incident solar power [W/m^2]**	**Weather Conditions**	**Spectral distribution**
Outside Atmosphere	-	1365	-	AM0
surface	a=90^o(Zenith)	925	Optimum	AM1
surface	a=48^o	963	USA average	AM1.5
surface	a=60^o	691	Average	AM2

Table1.1. Conditions for spectral distribution of Solar energy [data after Ref 2,3,4]

1.2 Fundamentals of Solar Cells

We know that carriers can be excited by thermal energy or heat and to produce electron hole pairs EHP's atoms can be ionized and there is one more way to give energy to materials is photons thus light.

In PN junction generated carriers that is minority carriers will be swept across the junction due to the presence of the electrostatic field across the depletion region thus, the excess electrons that is negative charge would collect in the n–type semiconductor and similarly, an excess of holes that is positive charge would collect in the p–type semiconductor. These excess carriers' electrons in n-type and holes in p-type will develop a differential voltage across the two sides of the device (figure 1.2). If we connect resistor across the device, current will flow from p to n region in outside circuit of device, this happening is known as photovoltaic.

To create an electron hole pair (EHP) in semiconductor, we require minimum quantity of energy which is equal to band gap Eg of semiconductor. A photon having energy less than band gap Eg and entering the cell then it will not absorbed by material and will pass through this material. A photon having energy equal to band gap energy is ideal to generate electron hole pair (EHP), so as the number of photons entering in the material increases number of electron hole pair generated increases. Hence photocurrent increases, photon having high energy would generate electron hole pair EHP offering energy equal to band gap Eg of material and dissipate the remaining amount of energy as heat. Those carriers which do not recombine before reaching the contacts contributes in the current but its disadvantage is lower maximum efficiency which is about 30 %, in practical maximum efficiency is only approx. 25%. (Data after Ref. [5])

The voltage is the result of photocurrent and diode current, thus current equation is written as

$$I = I_o \left[exp\left(\frac{qV}{nkT} \right) - 1 \right] - I_{PH} \quad \text{.....(i)}$$

Where, $I_d = I_o \left[exp\left(\frac{qV}{nkT} \right) - 1 \right]$ is diode current

Diode dark current depends on biasing of pn junction, V=forward voltage biasing, k= Boltzmann constant, T= temperature in Kelvin.

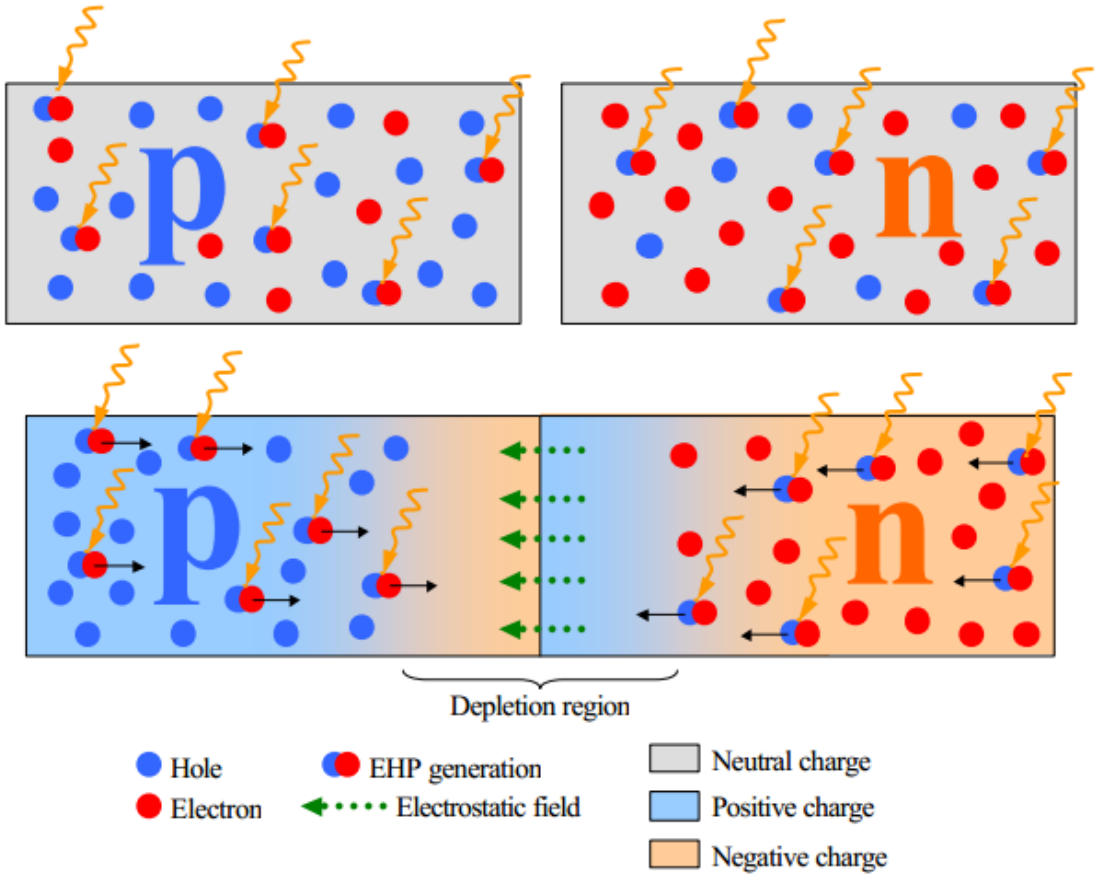


Fig. 1.2 Schematic of p–n junction formation (data after Ref. [6])

Open circuit voltage is the maximum voltage available at zero total current from the solar cell or open circuit voltage is equal to forward bias of solar cell until total current is zero in the circuit, it can be obtain by solving equation 1 for total current equal to zero.

$$I_{PH} = I_o \left[exp\left(\frac{qV}{nkT} \right) - 1 \right]$$

$$exp\left(qV / nkT \right) = \left(\frac{I_{PH}}{I_o} \right) + 1$$

$$V_{oc} = \frac{nkT}{q} exp \left\{ \left(\frac{I_{PH}}{I_o} \right) + 1 \right\}$$

The short-circuit current is simply a maximum photo generated current which can be drown from solar cell when voltage is zero. It is due to generation, recombination and collection of photo generated carriers, short circuit current is denoted by I_{sc} which depends on area of solar cell, number of photons, spectrum of incident light, band gap of material used, collection probability etc.

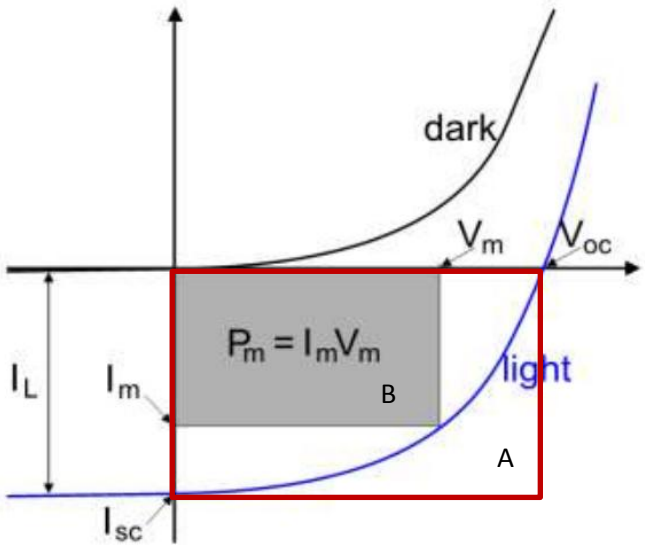


Fig 1.3 voltage and current relation of a single junction solar cell dark current (black) and photo generated current (blue) (data after Ref. [7])

Fill factor of solar cell is a measure of maximum product of current and voltage rectangle. At maximum voltage that is open circuit voltage V_{OC} and short circuit current I_{SC} power is zero as shown in the fig. 1.3 we have to find out the product of current and voltage starting from I_{SC} and voltage zero to V_{OC} and current zero. Fill factor commonly known by abbreviation “FF”.

$$FF = \frac{Area\ B}{Area\ A}$$

$$FF = \frac{I_M V_M}{I_{SC} V_{OC}}$$

Efficiency is most important parameter for comparing performance of one solar cell to another and it is defined as ratio of output energy to the input energy given to the solar cell and we know that fraction of input energy converted into electrical energy is defined as:

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

P_{max} = maximum converted power

We can calculate efficiency of solar cell by calculating the ratio of output power to the input power as:

$$\eta = \frac{V_{OC} I_{SC} FF}{P_{in}}$$

Where, η = efficiency

P_{in} = input power

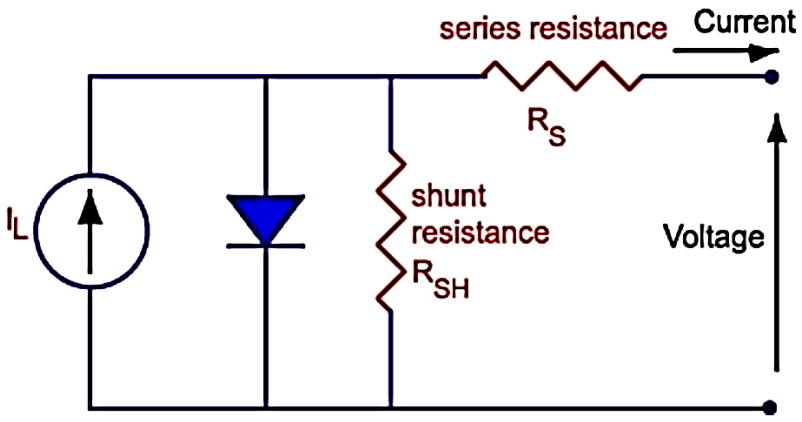


Fig 1.4 Parasitic shunt and series resistances in solar cell circuit (data after Ref. [8])

Series resistance effects fill factor of solar cell and its excess value may reduce short circuit current. Its ideal value is zero and main cause is the contact resistance between metal contact and semiconductor material; it reduces the current in solar cell which may be represents as:

$$I = I_{PH} - I_o exp\left[\frac{q\left(V + IR_S\right)}{nkT}\right]$$

Where, I = solar cell output current

R_S = series resistance of solar cell

I_{PH}= photo generated current in solar cell

Shunt resistance is main cause of power loss in solar cells if it is low in value it gives alternative path to photo generated current in solar cell it is due to manufacturing defect or poor manufacturing of solar cell and effect of shunt resistance is severe in low light intensity. Ideal value of shunt resistance is infinite Current of solar cell with shunt resistance can be written as:

$$I = I_{PH} - I_o exp\left[\frac{qV}{nkT}\right] - \frac{V}{R_{SH}}$$

If we consider both series and shunt resistance the current equation of solar cell is written as:

$$I = I_{PH} - I_o exp\left[\frac{qV}{nkT}\right] - \frac{V + I_{RS}}{R_{SH}}$$

Where, k (Boltzmann constant) = $1.38064 * 10^{-23} m^2 kg\ s^{-2} K^{-1}$

R_S = series resistance of solar cell

R_{SH}= shunt resistance of solar cell

1.3 Compound semiconductor (GaAs) or Si

As we know that solar spectrum has distributed from 250nm to 2500 nm as shown in fig.1.1 and we have different semiconductor material having different band gap between 0.36 to 3.5 eV, Such as InAs (0.36 eV), Si (1.12 eV), Ge (0.66 eV), InP (1.35 eV), GaAs (1.42eV), GaN (3.44eV), AlAs (2.16 eV), GaP (2.26 eV) PbS (0.37 eV), CdTe (1.49 eV), CdS(2.42 eV), CdSe (1.70 eV), and ZnO (3.35 eV) can absorb according to their band gap, lower the band gap material absorbs higher wavelength photons but as band gap of material reduces its open circuit voltage decreases because open circuit voltage cannot be greater than band gap of material. Based on Shockley and Queisser maximum efficiency limit for single junction solar cell is 31% (data after Ref. [9]).

If we compare between compound semiconductor material like Gallium Arsenide (GaAs) and simple indirect band gap semiconductor material silicon (Si), we know that Si is abundant on earth and industry is mature in its technology, purification and fabrication thus cheaper as compared to GaAs, but in optoelectronic properties silicon is not better than GaAs because gallium arsenide has direct band gap hence its absorption coefficient is higher than the absorption coefficient of silicon so, solar cell made of silicon must be thicker (100 μ m) than solar cell made of gallium arsenide (4 μ m) to absorb light completely. The mobility of silicon (Si) is much lower than the mobility of gallium arsenide (GaAs) and due to this difference in mobility, results in a slower photocurrent diffusion and drift in silicon (Si) based solar cell. GaAs substrate and growth is costly thus high efficiency GaAs based solar cell can be used on satellites.

Compound semiconductor especially III-V group like GaAs are widely used in light emitting diode (LED), photo detector, lasers and solar cell, so future of GaAs is bright as compared to silicon (Si).

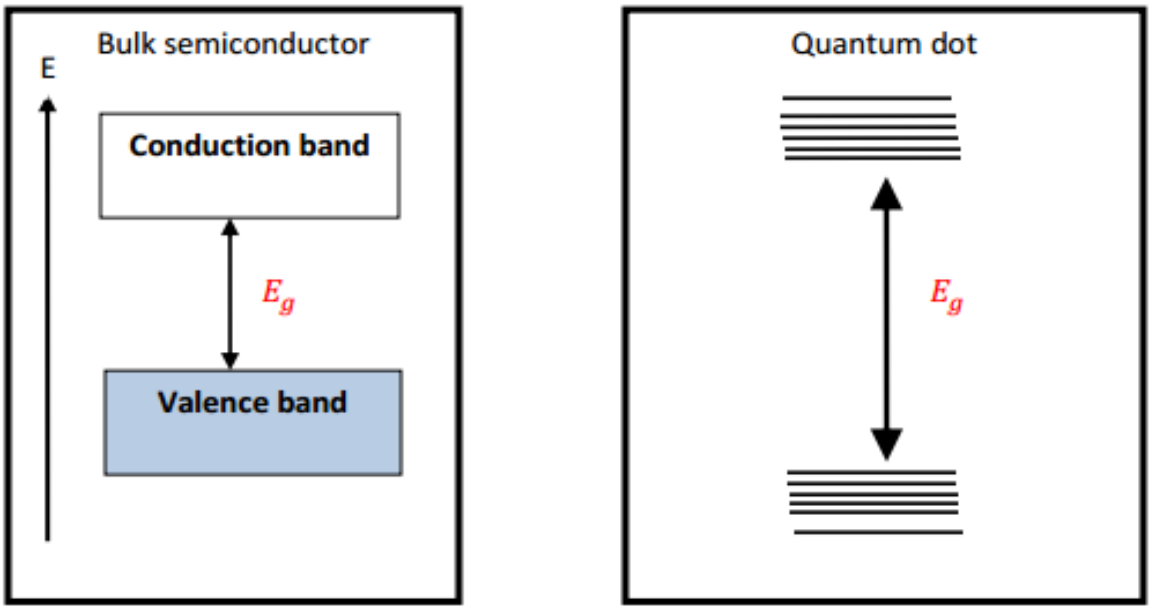
1.4 Efficiency improvement by nanostructure or multi-junction

The highest efficiency Shockley-Queisser limit of solar cell is 31% for single junction solar cell but practically GaAs based solar cell it is reached up to 28% which is near to the Shockley-Queisser limit. One way to increase efficiency is multi-junction tandem solar cell in which different semiconductor material having different band gap is connected with tunneling junction between two materials and these materials are connected in such a way that material having high band gap is above the structure and material having low band gap is connected at bottom of solar cell so that photons of higher wavelength will pass through higher band gap material and will be absorbed by low band gap material at bottom. Moreover it is limited by lattice match thus series of these material used in multi-junction is not free to choose. The maximum efficiency η_{max} of triple-junction solar cells GaInP/GaAs/GaInNAs has reached 43.5 % (data after Ref. [10]). In recent years nanostructure is hot topic for research like Quantum dots, quantum wells it gives new idea to improve efficiency as well as these nanostructure utilize hot carriers efficiently before these hot electrons relax to conduction band lower edge hence nanostructure are capable to increase photo currents and overall efficiency η_{max} of solar cell.

2. QUANTUM DOT (QDs) SOLAR CELL

2.1 Physics of Quantum Dots

A quantum dot is made up of semiconductor materials which is nanostructure that confines the motion of excitons (bound pairs of valence band holes and conduction band electrons) from all three special directions. These dots have discrete quantized energy spectrum. In a crystal of semiconductor whose radius is smaller than the size of its Bohr radius, the excitons are confined from all three directions. So, we can model the energy levels as a particle in a box in which the energy of states are dependent on the length of the assumed box. Quantum dots will be in the weak confinement regime if their radius is of the order of excitons Bohr radius and if their radius is smaller than the radius of excitons then these will be in the strong confinement regime. Size of quantum dots is typically from 1nm to 10nm. (Data after Ref.[11]). With the help of variations in quantum dots size we can get maximum efficiency.



Firure.2.1: Energy levels diagram for bulk semiconductor and quantum dot
(Data after Ref. [12])

Quantum Confinement depends on size of QDs and this occssurs when the size of the semiconductor QDs is equal to or smaller than the Bohr radius excitons, the electron in the conduction band and holes in the valence band are confined from all three dimensions of the material, this leads to discrete energy levels of semiconductor and band gap of semiconductor QDs increases as their size decreases.

As shown in figure.1 in bulk semiconductor energy bands are continuous but due to strong confinement in quantum dots (QDs) energy levels are in discrete in nature.

Size of quantum dots is smaller than as compared to working wavelength [13], we can also derive relation between its size and effective band gap with the help of basic quantum physics and effective mass of hole and electron, solving Schrodinger equation relation between the eigenvalue and energy level is

$$E= (h^2 * \beta^2)/ (2*m^*)$$

(Data after Ref. [14])

Where,

h = Plank's constant

β = eigenvalue

m^* = effective mass of electron (or hole)

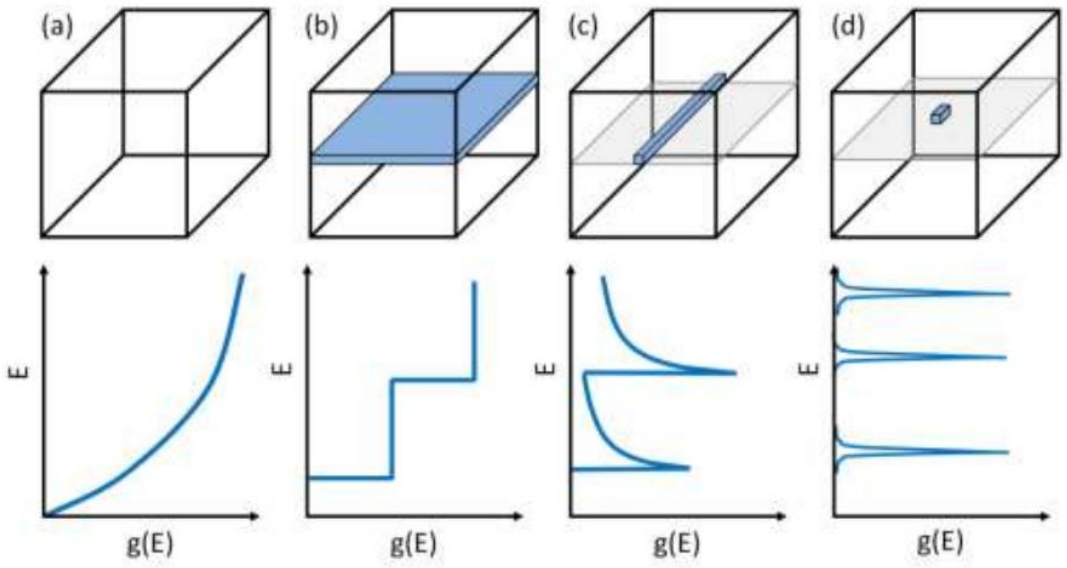


Fig.2.2 (a) Bulk material and its density of states, (b) Quantum well and its density of states, (c) Quantum wire and its density of states, (d) Quantum dot and its density of states (data after Ref.[15])

Fig 2.2 shows that density of energy states in the bulk semiconductor is continuous and it is quantized when we start confined any of three dimensions, here in Fig2.2 (d) showing quantum dot which is three dimensionally confined and energy state becomes completely discrete

2.2 Intermediate band solar cells (IBSCs)

As we know that efficiency of conventional solar cell is limited and it is totally dependent on band gap of material used in the solar cell. Photons having energy equal to band gap of semiconductor material is used very efficiently. Efficiency decreases as energy of photons increases greater than band gap of material because when energy is higher than band gap it produces hot electrons due to which extra energy dissipate as heat. Solar spectrum is broad thus we can observe this effect in single junction solar cell because this broad spectrum hardly matches band gap of material used in solar cell.

The main limitation of solar cell is low energy photons which cannot generate electron hole pairs and excite to conduction band, thus these photons does not contribute to the device current, and photons having high energy that is greater than band gap E_g of

material, due to a unmatched energy gap are not used efficiently in solar cell. If we introduce intermediate band between conduction band and valence band we can utilize in stepwise manner these low energy photons and it would be better matched to band gap of material.

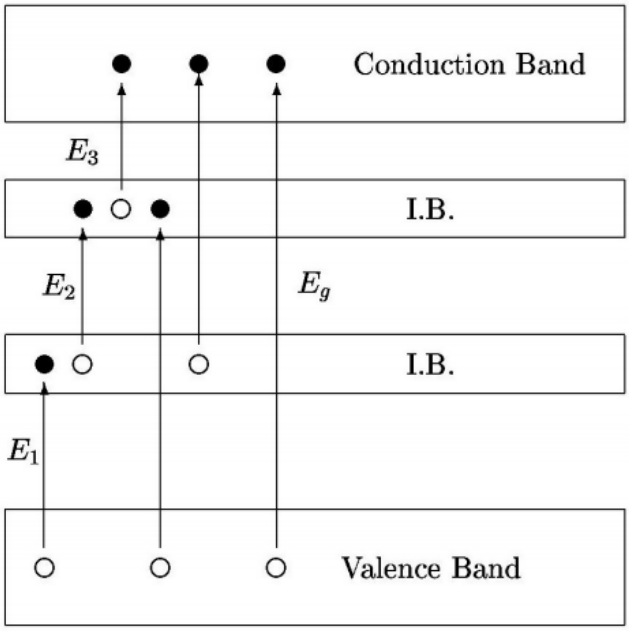


Fig.2.3 Two (IB) intermediate bands showing the all possible electronic transitions (data after Ref. [16])

In Fig 2.3 there are two (IB) intermediate bands between conduction and valence band and electron can excite from valence band to intermediate band, intermediate band to conduction band or directly valence band to conduction band. To calculate efficiency of IBSC there is some assumptions (data after Ref. [16, 17]) which we have to take i.e. Only radiative transitions between the bands occurs; One photon generates only one electron hole pair; From the intermediate band (IB) no carrier can extract; Mobility of carriers is infinite thus consequence is quasi-Fermi levels of energy are constant in the cell.

2.3 Quantum Dot (QD) Intermediate band solar cells

From previous sections it is clear that if we introduce intermediate band (IB) between the forbidden bands of solar cell it increases efficiency that is far superior compared to the efficiency of conventional device by absorbing low energy photons. Due to the advancement in micro-fabrication technology, today it is possible to grow more than two dissimilar semiconductors coherently which force quantum confinement to charge carriers; these types of structures where two materials are dissimilar is known as heterostructure (data after Ref. [18]). Heterostructure that confine carriers in three directions, two directions, and one direction are called quantum dots, quantum wires, and quantum wells respectively. In this section there will be a discussion on different types of heterostructure.

2.3.1 HETEROSTRUCTERS

A heterostructure consists of two or more than two different semiconductor materials that are grown on common crystal structure, but we have to care in these types of structure about band alignment of relative energy of different band gap of semiconductor materials. For example if we consider hetrostructers of compound semiconductor material Aluminum Arsenide (AlAs) and Gallium Arsenide (GaAs) that are alternatively connected one of the axis. As we know that band gap of pure semiconductor aluminum arsenide (AlAs) is higher than the band gap of gallium arsenide (GaAs). Band alignment is such that conduction band of gallium arsenide (GaAs) is below the conduction band of (AlAs) and valance band of gallium arsenide (GaAs) is above the valence band of aluminum arsenide (AlAs) due to this there is energy difference between the valence bands of AlAs and GaAs. This is known as valence band offset, similarly we can define conduction band offset.

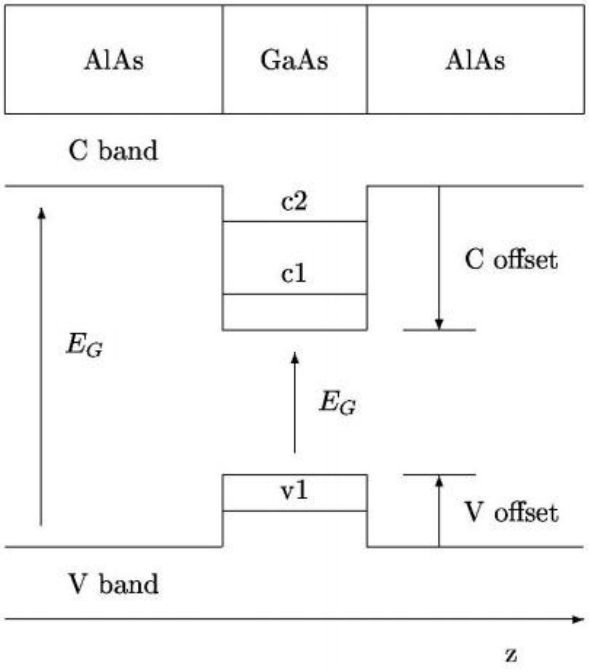


Fig 2.4 Semiconducting material GaAs and AlAs alternatively connected creates a heterostructure (data after Ref. [19, 20, and 21])

Energy levels that are between conduction and valence band of material known as intermediate bands (IB). Intermediate levels of quantum well provides state of finite energy density which are lying between the conduction and intermediate bands (IB) of material, which is due to the equation of energy spectrum; $\frac{\hbar^2(\kappa_x^2+\kappa_y^2)}{2\,m^*}$

Intermediate band (IB) which is lowest will act as a conduction band and the behavior of heterostructure will be a single energy gap (E_g) device (Data after Ref. [22, 23]).

But in quantum dot (QD) heterostructure, it provides zero density of states among the excited bands because of the spectrum of discrete energy and every band is thermally isolated from each other, Fermi level of material will split into number of bands and concentration of charge carrier in each of the splinted bands can be calculated by levels chemical potential which is required for the operation of intermediate band solar cell

(IBSC). It will minimize dissipation of extra energy as a heat in device that is why QDs are used in IBSC for their physical realization.

2.4 InAs (QDs) embedded GaAs based solar cells

There is three layer structure shown in Fig.2.5 having lightly doped p and n-type semiconductor material in my structure there is gallium arsenide (GaAs) and quantum dots are of different material that is indium arsenide (InAs) surrounded by barrier material that is intrinsic gallium arsenide (GaAs). Spacing between and size of quantum dot should be uniform because it establish good boundaries of intermediate band (IB). If these dots would not be symmetric then energy level would never be equally spaced (Data after Ref. [24]). If there would be size variation between these quantum dots then also energy level would never be equally spaced.

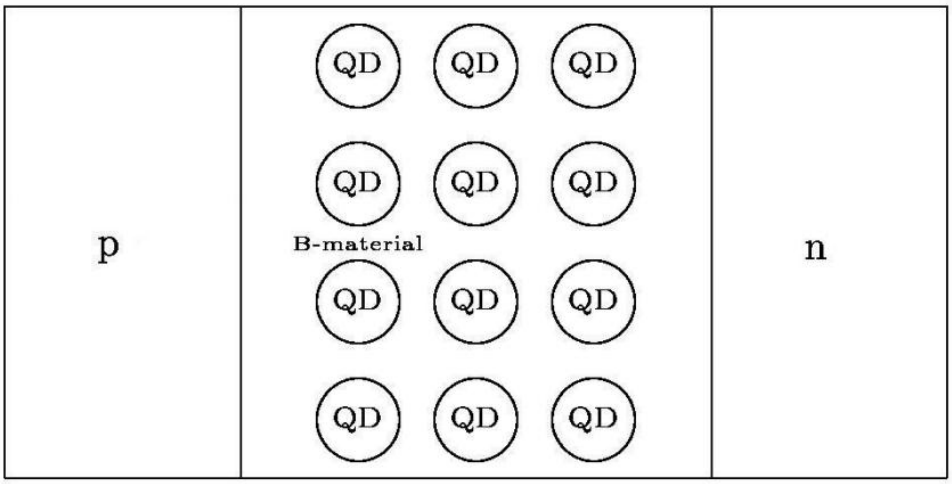


Fig. 2.5 Proposed Quantum Dot (QD)-Intermediate Band Solar Cell (IBSC) in the intrinsic layer surrounded by barrier material and these are arranged periodically (Data after Ref. [25])

Position of quantum dot layer in intrinsic layer of structure is also important for getting extra photocurrent in infrared region because of which external quantum efficiency (EQE) increases, most of the electron hole pairs generate at intrinsic layer. Quantum dots should be placed very close to each other in the intrinsic layer to form continues intermediate band (IB) (Data after Ref. [26])

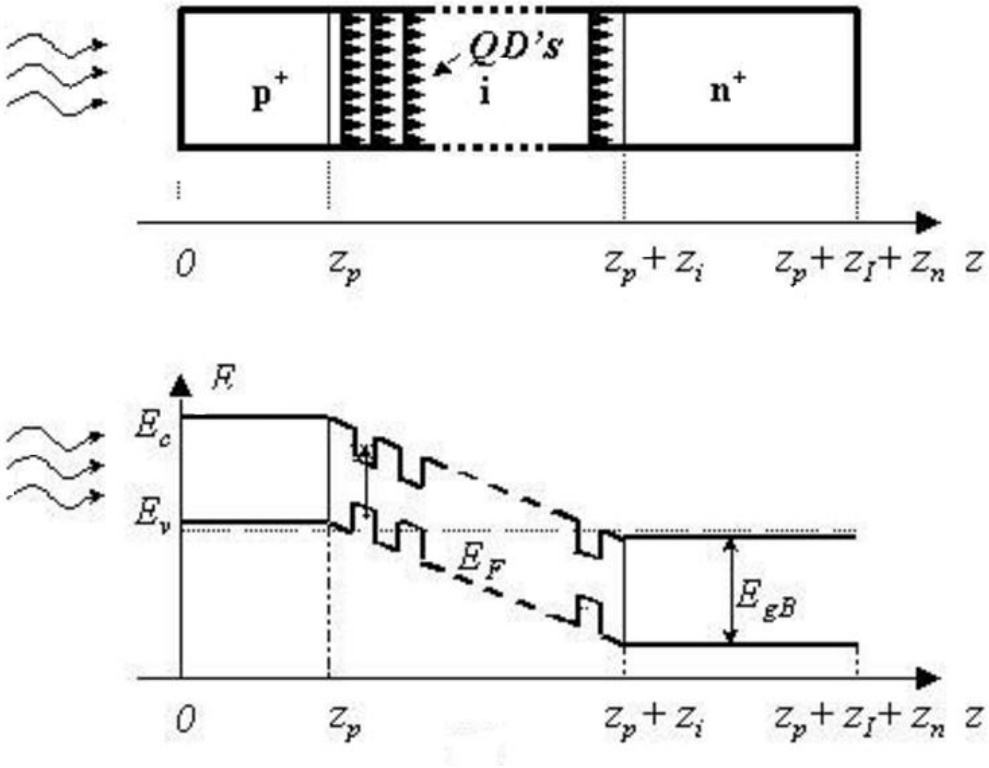


Fig. 2.6 Band diagram of *pin* solar cell with QD in intrinsic layer (Data after Ref. [27])

In Fig. 2.6 there is highly doped p and n type material and intrinsic layer is embedded between these two regions with quantum dot showing degenerate p-type semiconductor from 0 to Z_p, intrinsic layer of width Z_i with quantum dot at regular interval embedded between barrier material that is intrinsic semiconductor and degenerate n-type semiconductor of width Z_n

III. SILVACO ATLAS

In this method and strategy for modeling solar cell using Silvaco atlas TCAD software is discussed. Silvaco is a company that gives platform for creation of simulation software comprising almost every aspect of modern electronic design. It provides tools to create complex models and 2D, 3D structures. A wide variety of material properties (e.g., optical parameters, recombination parameters, mobility, ionization coefficients) leads to the accuracy of the device simulation.

The order of statements occurs in ATLAS is important, There are five group of statements which must be in correct order (Fig. 2.1)

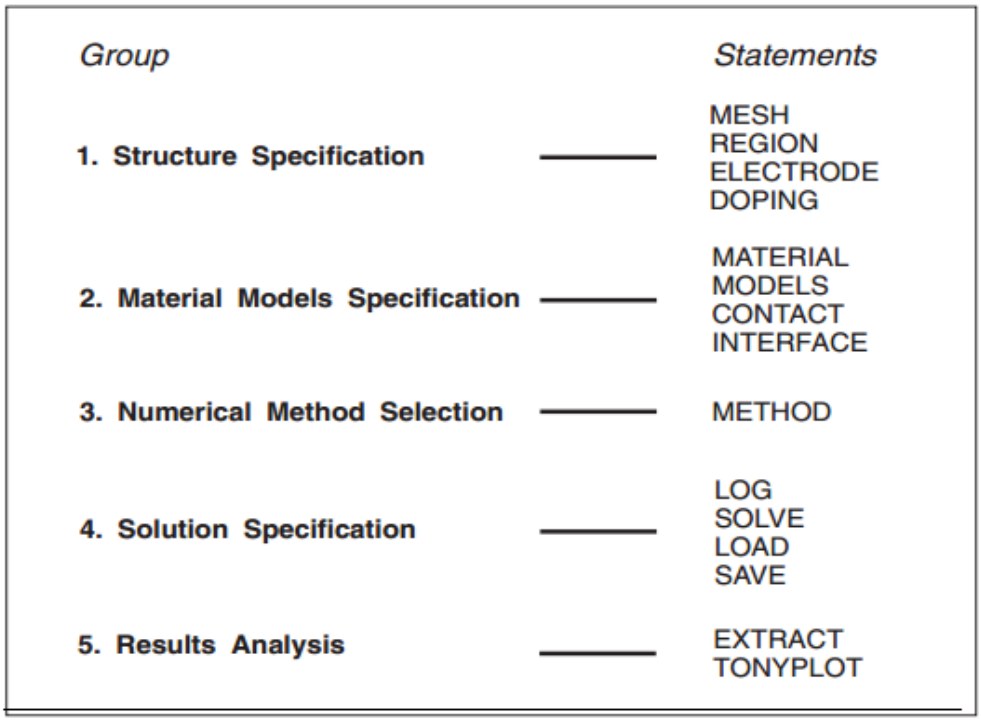


Fig. 3.1 ATLAS Command Groups with correct order (data after Ref**. [28])**

3.1 MESHING

First thing that has to be done is meshing, several constants and specification can be done in the meshing declaration in the ATLAS, specification should be correct in order to the final accuracy of results, if the number of triangle density is not enough then final result will not be accurate and on other side if number of triangles is too large then also results of simulation will take more execution time. Meshing at junctions where we want large number of solution during simulation should be large; here is an example of meshing which is used during simulation. In x direction it is large as compared to y direction.

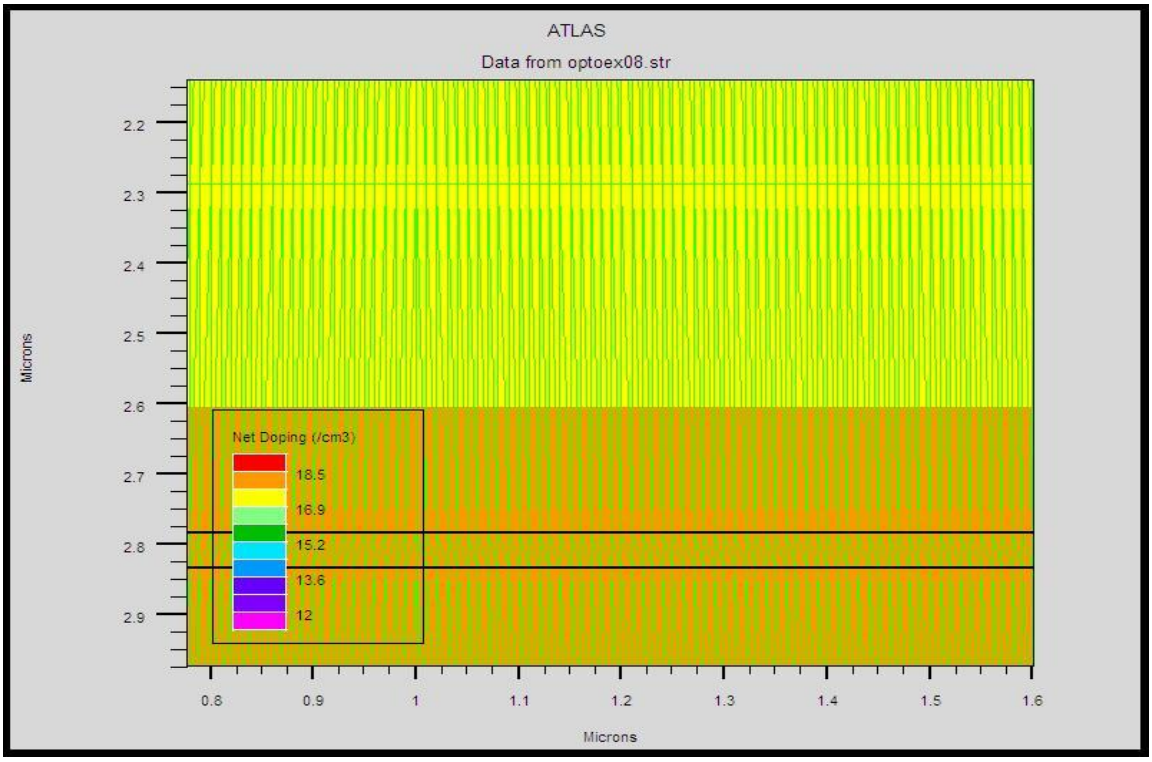


Fig. 3.2 Meshing in structure

X.MESH LOCATION=<VALUE> SPACING=<VALUE>

Y.MESH LOCATION=<VALUE> SPACING=<VALUE>

When specifying meshing in x direction we prefer less spacing at center but in y direction spacing usually change at every region

In this simulation meshing is specified by following command as given below

In x direction by commands

SECTION 1: Mesh Specification

```
mesh space.mult=1.0
#
x.mesh loc=0.00  spacing=0.01
x.mesh loc=0.01  spacing=0.01
x.mesh loc=0.02  spacing=0.01
,,,,,,,,,,,,,
,,,,,,,,,,,,,

x.mesh loc=1.97  spacing=0.01
x.mesh loc=1.98  spacing=0.01
x.mesh loc=1.99  spacing=0.01
x.mesh loc=2.00  spacing=0.01
```

In the y direction by the commands,

```
y.mesh loc=0.0       spacing=0.05
y.mesh loc=0.05      spacing=0.05
y.mesh loc=0.55      spacing=0.1
```

loc=0.55 to loc=0.7850 Quantum Dots specifications

```
y.mesh loc=0.7850    spacing=0.05
y.mesh loc=2.7850    spacing=0.5
y.mesh loc=2.8350    spacing=0.1
y.mesh loc=3.0850    spacing=0.5
```

Here, location is in micron (10^{-6}m)

3.2 REGIONS

The regions of material need to be specify in the next step. Here, all grid parts to a specific material are assigned (Figure 2.3). It can be selected from Silvaco's library or it can be defined by the user. Quantum Dots grading between intrinsic regions in the structure is also described. Maximum number of regions that ATLAS allows is 55 (fifty), this is the limiting factor of silvaco.

The positions of the regions are specified in both directions with the commands specified in atlas x.min, x.max, y.min and y.max.

REGION NUM=<VALUE> MATERIAL=<VALUE> X.MIN=<VALUE> X.MAX=<VALUE> Y.MIN=<VALUE> Y.MAX=<VALUE>

In this simulation regions is specified by command as following

```
# SECTION 2: Structure Specification
#
region num=1   material=InGaP   x.min=0.0   x.max=2.0   y.min=0.00     y.max=0.05
region num=2   material=GaAs    x.min=0.0   x.max=2.0   y.min=0.05     y.max=0.55
region num=3   material=GaAs    x.min=0.0   x.max=2.0   y.min=0.55     y.max=0.5850
region num=4   material=GaAs    x.min=0.0   x.max=2.0   y.min=0.5850
y.max=0.5865
region num=5   material=GaAs    x.min=0.0   x.max=2.0   y.min=0.5865
y.max=0.5915
```

Quantum Dot (QDs) layers region specifications

```
region num=51 material=GaAs    x.min=0.0   x.max=2.0   y.min=0.7850
y.max=2.7850
region num=52 material=InGaP   x.min=0.0   x.max=2.0   y.min=2.7850
y.max=2.8350
region num=53 material=GaAs    x.min=0.0   x.max=2.0   y.min=2.8350
y.max=3.0850
```

3.3 ELECTRODES

After specifying regions next step is to specify where the current will collect by the electrode command. The electrodes are located at top and bottom. The position parameters are very similar to specify in regions.

ELECTRODE NAME=<electrode name> <position parameters>

In this simulation, electrodes are found only at the top and the bottom of the solar cell and they are specified by the following commands:

Electrode name = cathode top

Electrode name = anode bottom

```
#
elec num=1 name=anode x.min=0.0 x.max=2.0 y.max=0.0
elec num=2 name=cathode bottom
```

3.4 DOPING

Doping is necessary in semiconductor to make it n-type or p- type. In silvaco tcad there is no limit of doping of semiconductor, it also allows us to do various type of doping like Gaussian, uniform and in this simulation we use uniform type doping by command

```
#Doping
#
doping uniform conc=2e18 p.type  x.min=0.0  x.max=2.0  y.min=0.0000    y.max=0.05
doping uniform conc=1e18 p.type  x.min=0.0  x.max=2.0  y.min=0.0500    y.max=0.55
doping uniform conc=1e17 n.type  x.min=0.0  x.max=2.0  y.min=0.7850  y.max=2.7850
doping uniform conc=1e18 n.type  x.min=0.0  x.max=2.0  y.min=2.7850  y.max=2.8350
doping uniform conc=1e18 n.type  x.min=0.0  x.max=2.0  y.min=2.8350  y.max=3.0850
```

3.5 MODELS

This section describes the models which is used in this simulation

1. Model based on Low field mobility which is used for calculations of the mobility of carriers depending on temperature

$U_{n0}(T_L) = MUN *(T_L/300)^{TMUN}$

$U_{p0}(T_L) = MUN *(T_L/300)^{TMUN}$

2. Model based on Concentration which is used for calculation of the mobility of carriers depending on concentration, and which is given by Masetti model [29]

$U_n = U_{nmin}*\exp(-P_{c.n}/N_D) +\{(U_{nman}- U_{nmin})/1+(N_D/C_{r.n})^{a.n}\}-\{(U_{1.n})/1+(C_{s.n}/ N_D)^{B.n}\}$

$U_p = U_{pmin}*\exp(-P_{c.p}/N_A) +\{(U_{pman}- U_{pmin})/1+(N_A/C_{r.p})^{a.p}\}-\{(U_{1.p})/1+(C_{s.p}/ N_A)^{B.p}\}$

3. SRH-Shockley-Read-Hall recombination model using lifetimes depending on concentration it is used to calculate of carrier's recombination, which is given by the equations given below,[30]

$R_{SRH} = (pn-n_i^2) / \{t_{n*}(n+n_i*\exp(ETRAP/KT_L)) + t_{P*}(p+p_i*\exp(-ETRAP/KT_L))\}$

4. Self-Consistent Coupled Schrödinger Poisson model for the effects of quantum confinement which is given for 2D confinement by the following equations:

$(-h^2/2)*d/dx\{(1/m_e^*)*(d/dx(si))\} + E_c(x)*si = E_i*si$

$(-h^2/2)*d/dx\{(1/m_h^*)*(d/dx(si))\} + E_v(x)*si = E_i*si$

Command: models ,,,,,,,,,,,,,,,,,,schro.2dxy

Some models which requires at heterojunctions between InAs quantum dot and GaAs intrinsic semiconductor like Stark Effect, tunneling is included.

3.6 BEAMS AND METHODS

Lightening is important for solar cell device photo generation rate depends on light, silvaco provides variations in light source and to adjust source location, intensity and orientation. Polarization, reflectivity features are also important parameters for best results. Here we have used command for light beam at 90^o angle as

Beam num=<value> x.origin=<value> y.origin=<value> angle=<angle> file=file name

beam num=1 x.origin=1.0 y.origin=-2.0 angle=90.0 power.file=optoex08.spec

Methods use for convergence newton iteration method.

A material property also has to be specified in simulation. There are predefined properties of semiconductor materials. Here is table for some semiconductor materials

material	Lattice constant. [angstrom]	Permittivity [e_e/e_o]	Affinity [eV]	electron effective mass (m^*/m)	hole effective mass (m^*/m)	MUN mobility cm2/Vs	MUP Mobility cm2/Vs
Si	5.43	11.9	4.17	0.92	0.54	1500	500
GaAs	5.65	13.1	4.07	0.063	0.5	8800	400
InAs	6.06	14.6	4.54	0.021	0.43	33000	450

Table 3.1 Major parameters for unary and binary materials (data after Ref. [31])

IV. RESULTS AND DISSCUSSION

On increasing intrinsic layer between p and n-type material we observed as we are increasing our intrinsic layer width, short circuit current of device is increasing change in open circuit voltage of device is very low. In Fig.4.1 0 to 0.45um there is p-type semiconductor and 0.45um to 2.45um is n- type. Material shown in red color is high doping Indium Gallium Phosphide (InGaP) for reducing series resistance of solar cell and this series resistance effects short circuit current of device which should be ideally zero.

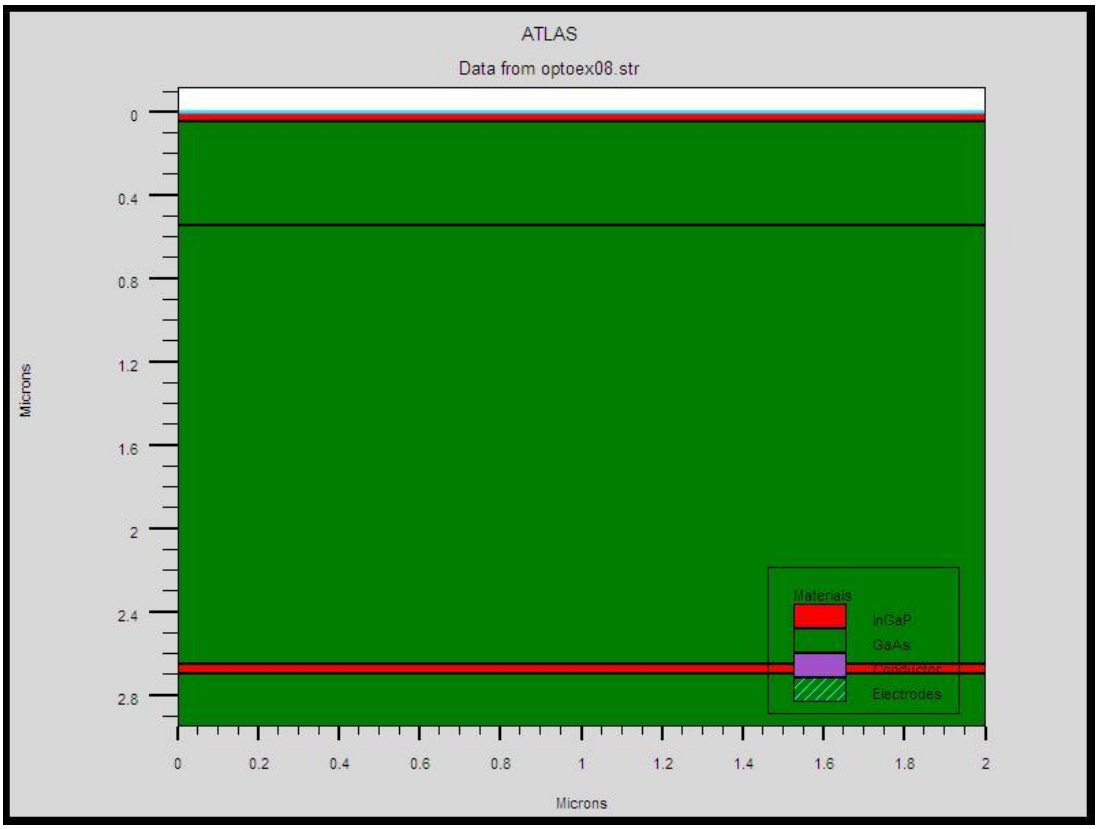


Fig.4.1 p-n junction solar cell structure having no intrinsic layer

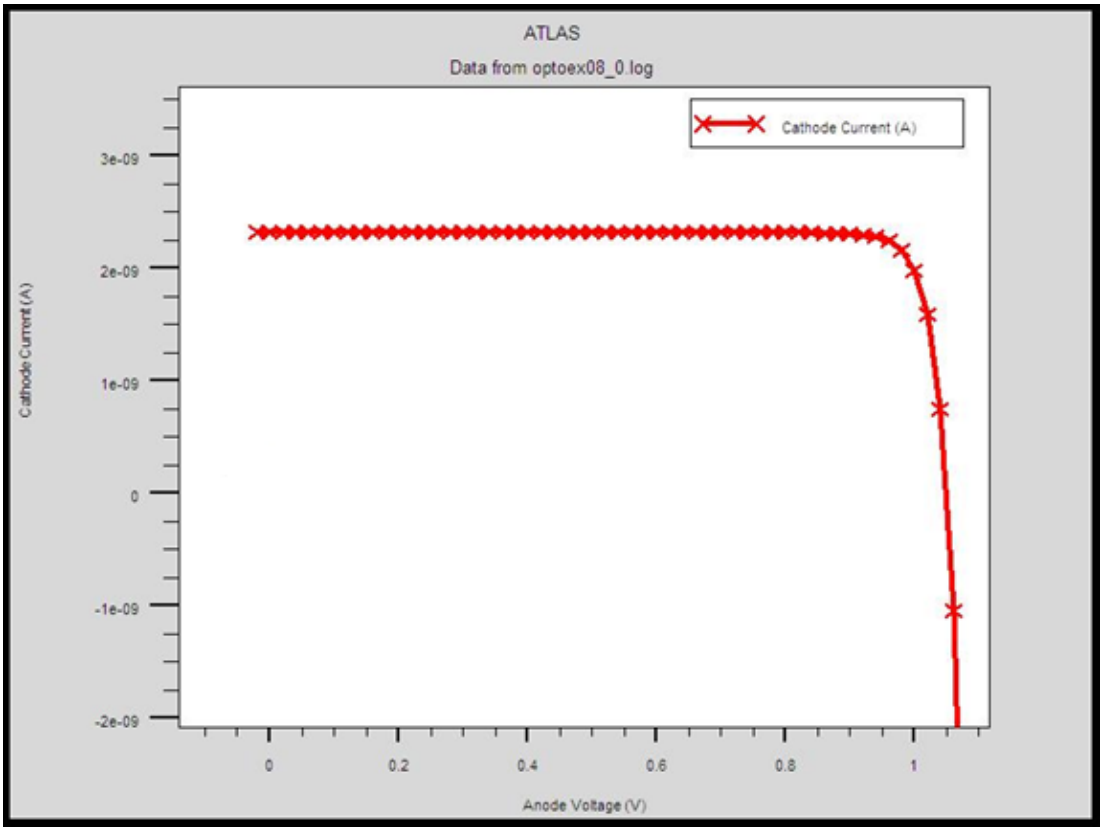


Fig 4.2 IV characteristics of solar cell having no intrinsic layer

In Fig.4.2 current and voltage characteristics of solar cell is obtained from Tony Plot of Silvaco software when there was no intrinsic layer only p-type and n-type semiconductor i.e. GaAs was there, from this graph we can obtain its short circuit current when anode voltage is zero and open circuit voltage when short circuit current is zero.

Open circuit voltage V_{OC} = 1.0485 V

Short circuit current density J_{SC} = 23.1431 mA/cm^2

Maximum power = V_{OC}*I_{SC} = 23.1431*1.0485 = 24.26554035 mW

Fill Factor = (21.567*0.95 = 20.9199) / 24.26554035

= 0.862123

Efficiency η % = (20.9199 mW / 100mW)*100

= 20.9199 %

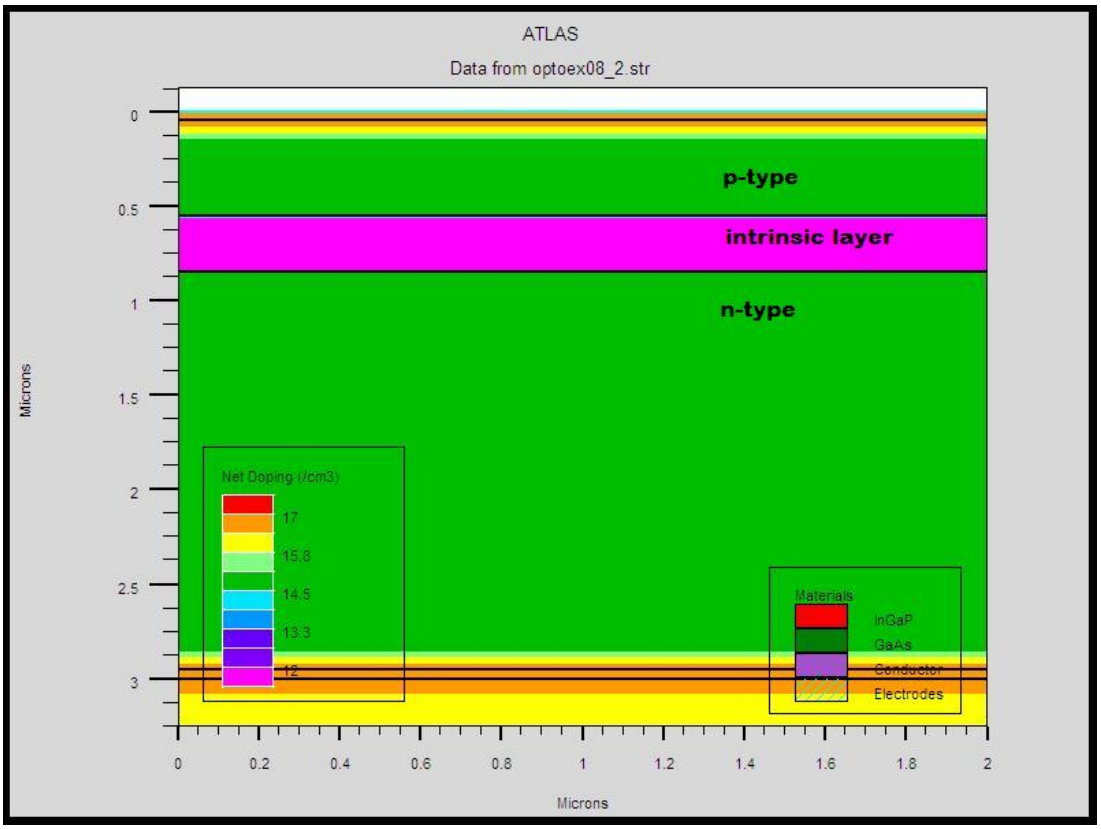


Fig.4.3 p-n junction solar cell structure having 0.3um intrinsic layer

In Fig.4.3 there is intrinsic layer between p and n-type GaAs showing pink in color which is also showing that doping of this pink region is of below 10^{12} and above p-type material there is InGaP which is highly doped showing in red and brown color for making contact resistance that is series resistance low. At the top of structure there is blue color showing opaque contact material so that light falling on device at 90 degree can enter inside the solar cell.

In Fig.4.3 current voltage i.e. IV characteristics of three different structures of solar cell is compared red one is for structure in which we have not used intrinsic layer, green curve is for introducing intrinsic layer of thickness 0.3um between p and n-type GaAs and making p-i-n structure and third one blue is for intrinsic thickness 0.8um. We found that short circuit current increased but open circuit voltage remains almost constant.

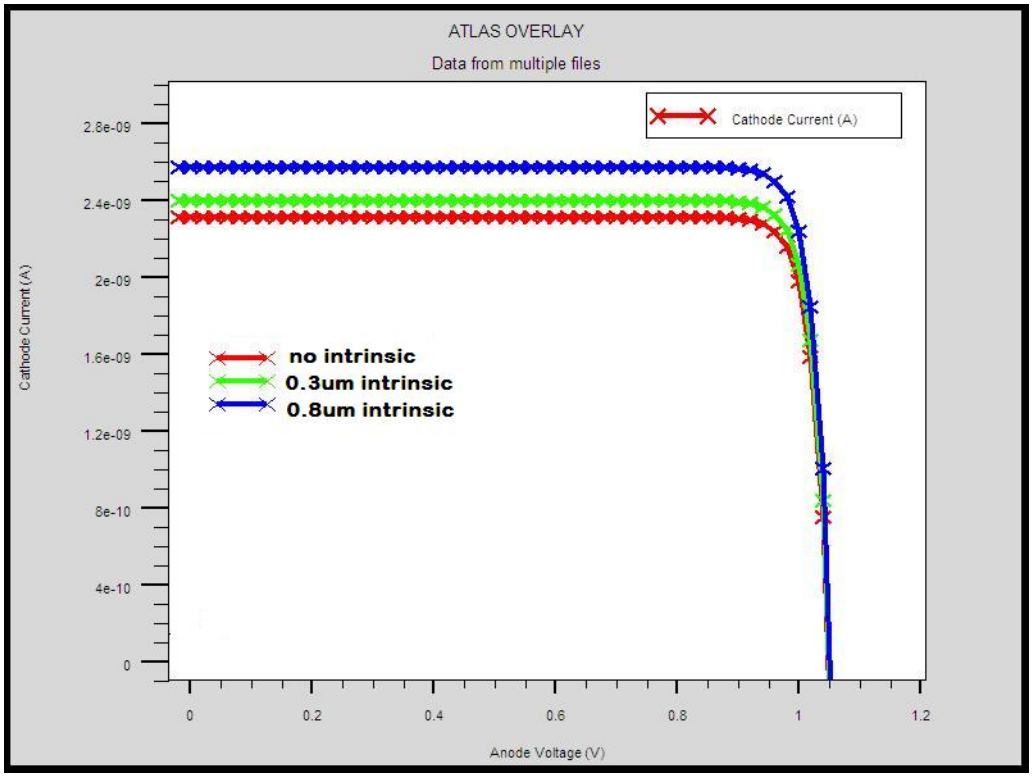


Fig.4.4 IV curve of solar cell structure having 0, 0.3um and 0.8um intrinsic layer

We can find out individual structure's open circuit voltage and short circuit voltage can find out their efficiency as shown in table;

Intrinsic width	Open circuit voltage V_{OC} (V)	Short circuit current density J_{SC} (mA/cm^2)	Efficiency η %
Zero	1.0485	23.143	20.92
0.3um	1.0494	24.081	22.02
0.8um	1.0512	25.739	24.72

Table 4.1 Showing increase in short circuit current, open circuit voltage and efficiency

However, we can see the change in open circuit voltage in Fig4.4 showing that open circuit voltage is increasing very small on increasing width of intrinsic layer but short circuit current is increasing very large.

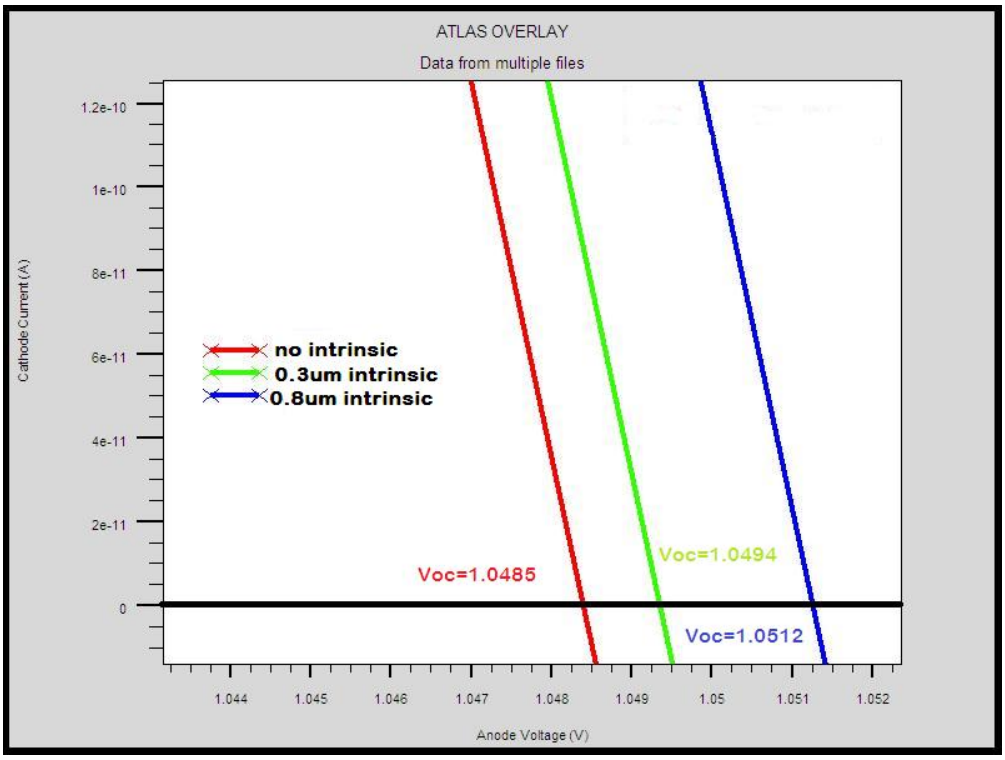


Fig 4.5 change in open circuit voltage on increasing intrinsic layer width

For finding the effect of intrinsic layer width on External quantum efficiency (EQE) of solar cell, we simulate solar structure shown in Fig.4.5

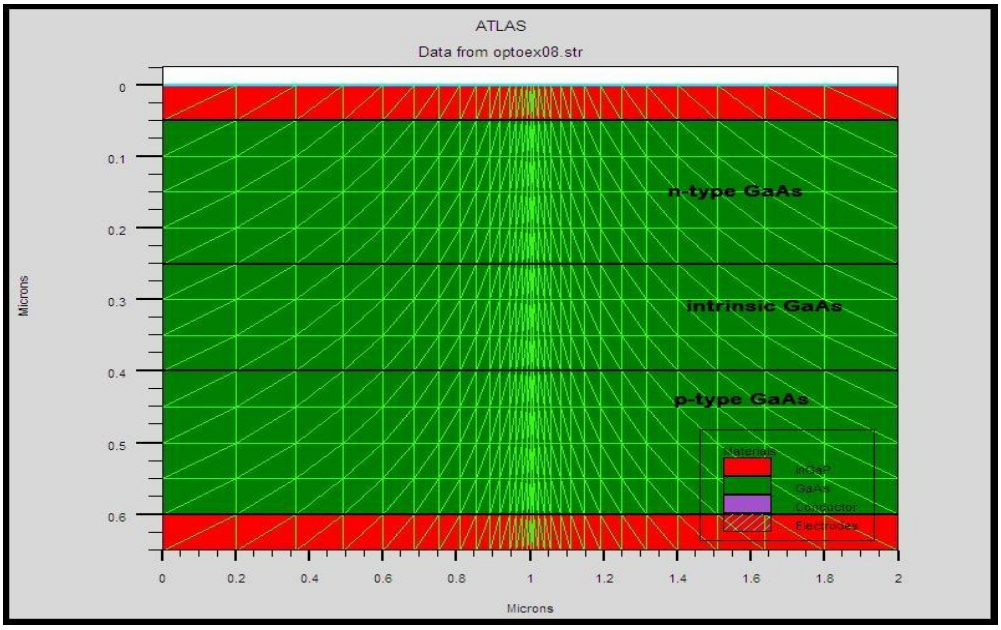


Fig. 4.6 structure of *pin* solar cell (data after Ref. [32])

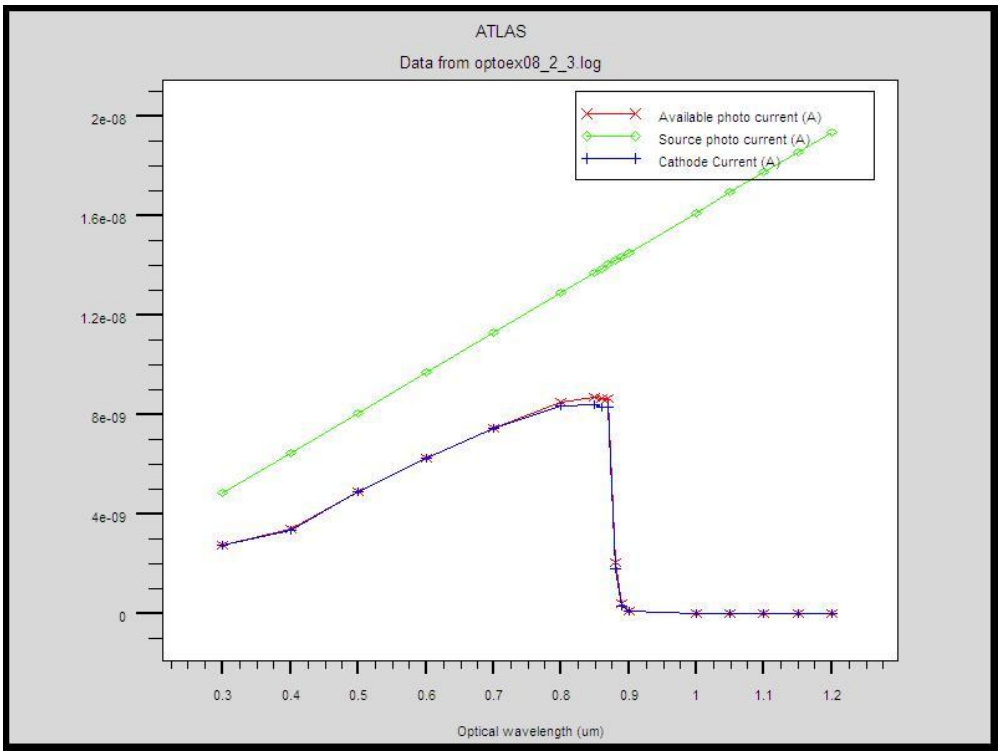


Fig.4.7 showing cathode current variation with optical wavelength

In Fig. 4.6 it is shown that as wavelength of light increases cathode current increases but at 0.87um it sharply goes to very low nearly zero because cut off wavelength of GaAs is 870nm. In red color there is available photo current in solar cell, in green color showing source photo current in amperes (A) and in violet color is cathode current of solar cell. We can calculate internal or external quantum efficiency of solar cell with this graph like,

$$\text{External Quantum Efficiency (EQE)} = \frac{\text{cathode current}}{\text{source photo current}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(i)}$$

$$\text{External Quantum Efficiency (EQE)} = \frac{\text{availabe photo current}}{\text{source photo current}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(ii)}$$

(Data after Ref. [34])

After applying equation (i) we calculate EQE of structure in Fig.4.5 showing that on increasing thickness of intrinsic layer EQE increases.

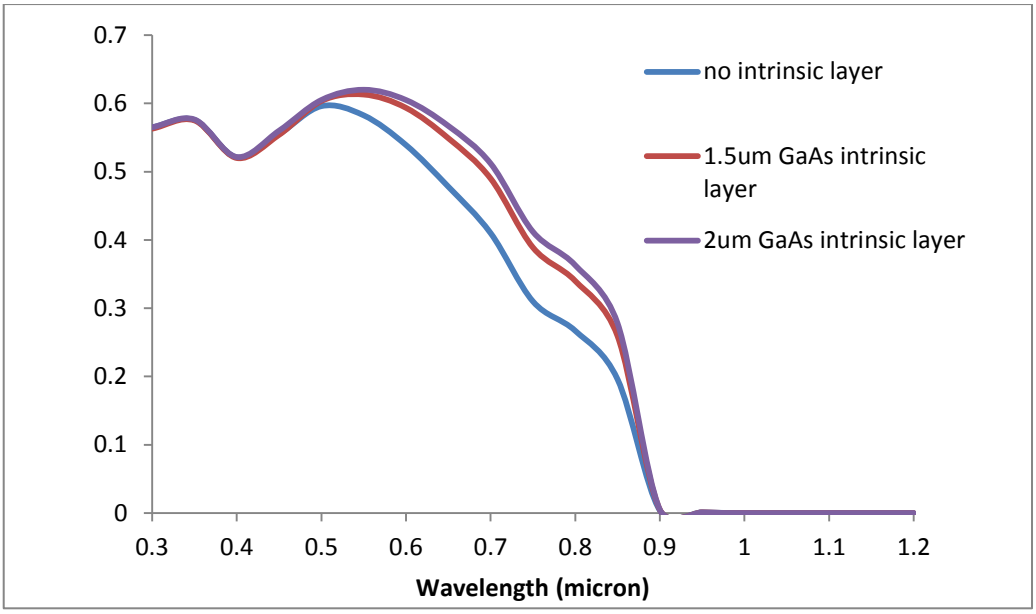


Fig.4.8 comparison of EQE of *pn* solar cell (blue) and *pin* solar cell (red and violate)

Here, in Fig. 4.7 there is three curve with wavelength varying from 300nm to 1200nm on x axis of graph blue is showing simple p-n junction solar cell's EQE having no intrinsic layer, red and violet showing pin structure of solar cell in which intrinsic layer are of a.5um and 2um respectively and showing increase in EQE.

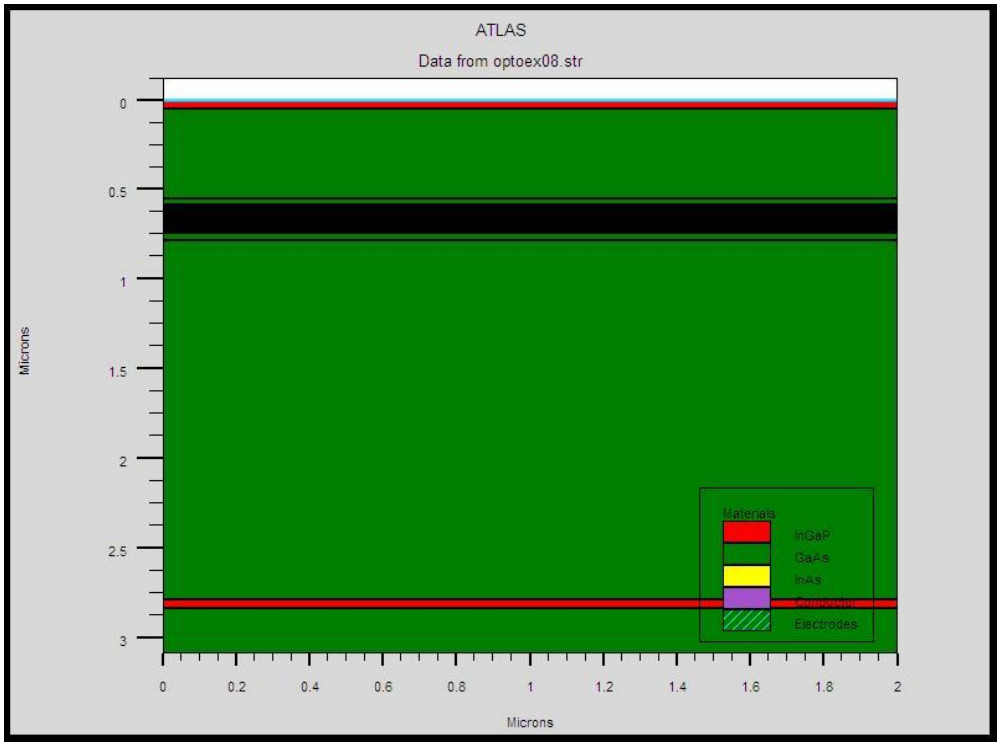


Fig 4.9 Structure of pin with GaAs/InAs QDs solar cell

When we introduce quantum dots in structure as shown in Fig. 4.8, here in Fig4.9 Quantum Dots (InAs) structure in intrinsic layer of GaAs is shown i.e zoom part of intrinsic layer with quantum dot in above circuit diagram in which we took InAs of size Height= 5nm Width= 10nm and barrier material that is GaAs is of 15nm of thikness between two layers of quantum dots.

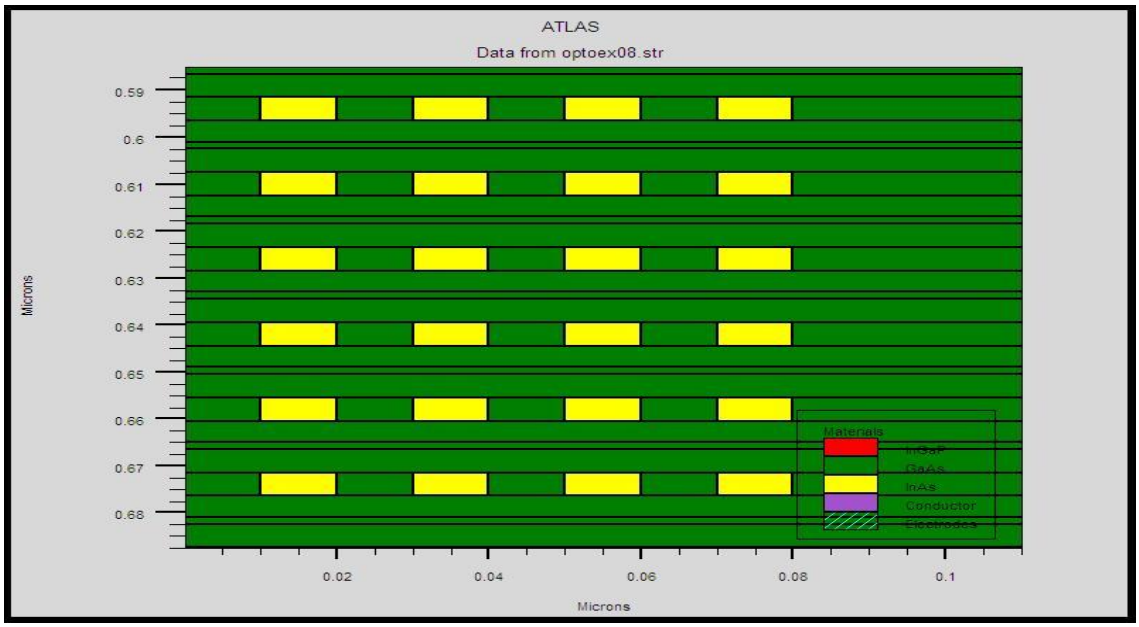


Fig 4.10 InAs (yellow) QDs in GaAs (green) intrinsic layer

Here,

Quantum Dots Height= 5nm Width= 10nm

After simulations results we found that by using InAs quantum dots in intrinsic region of GaAs external quantum efficiency increases in infrared region up to 1.2um of wavelength which was earlier only up to 870nm because photons having less energy than band gap of GaAs is absorbed by quantum dots InAs

After simulations results we found that by using InAs quantum dots in intrinsic region of GaAs external quantum efficiency increases in infrared region up to 1.2um of wavelength which was earlier only up to 870nm because photons having less energy than band gap of GaAs is absorbed by quantum dots InAs shown in Fig. 4.11

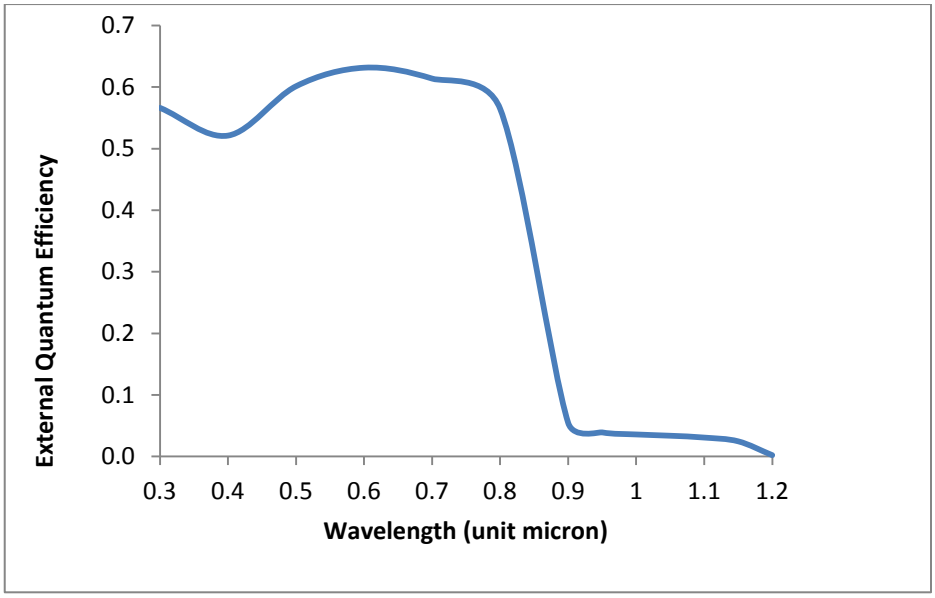


Fig.4.11 External quantum efficiency with InAs quantum dots (10 layers)

As conventional p-n junction solar cells have only p-type semiconductor and n-type semiconductor. Here we have introduced intrinsic semiconductor material (GaAs) between p and n type of semiconductor, due to which EQE increases up to cut off wavelength of GaAs and because of quantum dots of InAs having band gap lower than GaAs absorbs photon of lower energy increases EQE above cut off wavelength.

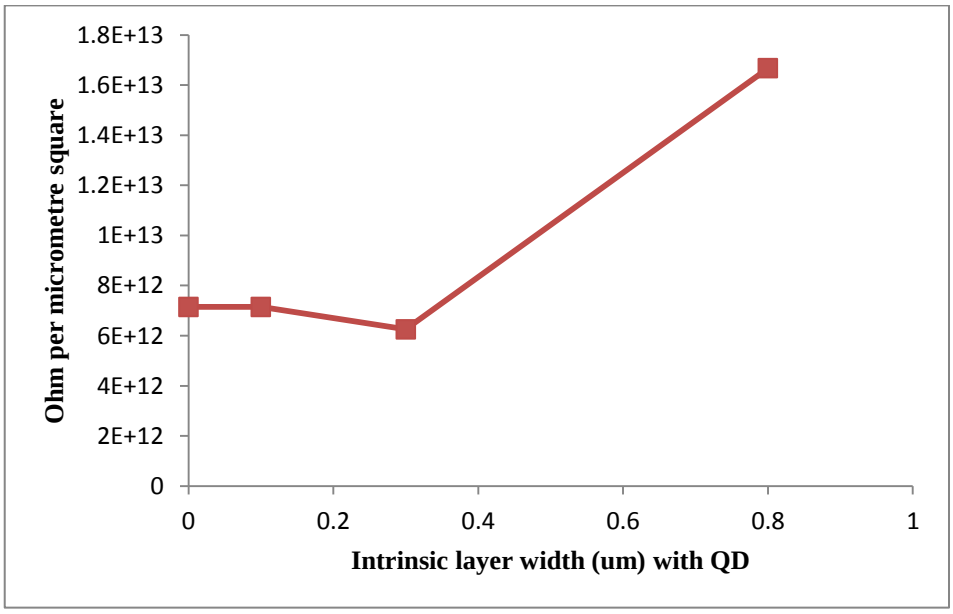


Fig 4.12 Shunt resistance of solar cell with intrinsic layer width with QD

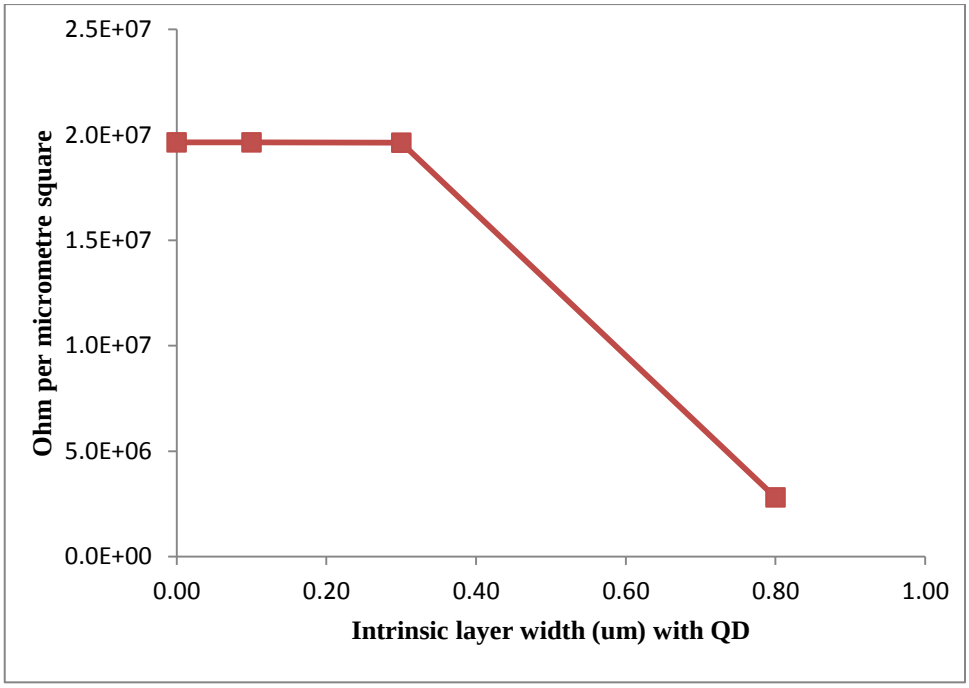


Fig 4.13 Series resistance of solar cell with intrinsic layer width with QD

In Fig 4.12 and Fig.4.13 shows that by increasing intrinsic layer with quantum dots, shunt resistance increases and series resistance decreases with increase width of intrinsic layer and quantum dot layers.

V. CONCLUSION AND FUTURE SCOPE

As we know that above cut off wavelength of semiconductor material which can absorb photon below its cut off wavelength, there is lot of energy that is wasted so, after using Quantum dots of semiconductor material we can absorb these energy as well as we can reduce extra energy of hot electrons that dissipate as a heat in solar cell which reduces its efficiency. Compared to the simple p-n junction solar cell *pin* structure solar cell increases its external quantum efficiency (EQE).

GaAs is a direct band gap semiconductor material thus its absorption coefficient is higher than indirect band gap semiconductor material like silicon (Si) and at one tenth of intensity of light output of GaAs remain constant but in silicon it decreases. As solar cell always place under sunlight thus it heats and in high temperature efficiency of silicon based solar cell decreases up to 30% but in GaAs based solar cell it remains constant, thus GaAs based solar cell can be used in printable solar cell, in satellites and all those places where humans cannot visit regularly.

REFRENCES

[1] Renewable Resource Data Center (rredc.nrel.gov).

[2] Sze, S. M., Semiconductor Devices, 2nd edition, John Wiley & Sons, Inc, 2001.

[3] Sze, S. M., Physics of Semiconductor Devices, 2nd edition, John Wiley & Sons, Inc, 1981.

[4] Shur, M. 1990. "Physics of Semiconductor Devices, Prentice–Hall".

[5]. "Photovoltaic Cell Conversion Efficiency Basics". U.S. Department of Energy.

[6]. Panayiotis M, 2002. A Novel Approach for the Development and Optimization of State-of-the-Art Photovoltaic Devices Using Silvaco

[7]. Jonathan D. 2011. "Patterned quantum dot for solar cell applications" University of Illinois at Urbana-Champaign.

[8].http://www.pveducation.org/pvcdrom/solar-cell-operation/impact of both resistances

[9]. Reinhardt K.C; Mayberry C.S; Lewis B.P; Kreifels T.L, 2000. "Multijunction solar celliso - junction dark current study", Photovoltaic Specialists Conference, Con ference Record of the Twenty - Eighth IEEE, pp 1118- 112

[10]. Modeling and Simulation of GaSb/GaAs Quantum Dot for Solar Cell "ARTICLE in ENERGY PROCEDIA" August 2015

[11]. http://www.sciencedaily.com

[12]. www.researchgate.net/publictopics.PublicPostFileLoader.html?id...key

[13]. Nakata, Y.; Y. Sugiyama, and M. Sugawara. 1990. "Molecular Beam Epitaxy Growth of Self-assembled InAs/GaAs Quantum Dots", Ch. 2, Academic.

[14]. Horiguchi, S. 1996. "Validity of effective mass theory for energy levels in Si quantum wires," Physics B, Vol. 227, Nos. 1–4, 336–338.

[15]. Leonid A. Kosyachenko, 2015. "Solar Cells-New Approaches and Reviews" ISBN 978-953-51-2184-8.

[16]. Luque, A.; Marti, A. 1997. "Increased efficiency of ideal solar cells by photon transitions at intermediate levels". Physical Review Letters, 78 (26).

[17]. Shockley, W.; Queisser. H.J. 1961. "Detailed and balance limit of the efficiency of p-n junction solar cells". Journal of Applied Physics, 32(3).

[18]. Kittel, C. 2005. “Introduction to Solid State Physics”. John Wiley and Sons, Hoboken.

[19]. Baskoutas, S. and Terzis, A. F. 2006. “Size-dependent band gap of colloidal quantum dots,” J. Appl. Phys., Vol. 99, No. 1, 013708.

[20]. Kasap, S. and Capper, P. 2006. “Handbook of Electronic and Photonic Materials”, 54–327, Springer.

[21]. Holmstrom, P.; L. Thylen, and A. Bratkovsky, 2010. “Dielectric function of quantum dots in the strong confinement regime,” J. Appl. Phys., Vol. 107, No. 6, 064307.

[22]. Anderson, N. G. 2002. “On quantum well solar cell efficiencies”. Physica E, 14:126–131.

[23]. Luque, A., Marti, A. 2001. “Thermodynamic consistency of sub-band gap absorbing solar cell proposals”. IEEE Transactions on Electron Devices, 49:2118–2124.

[24]. Gilmore, R. 2004. “Elementary Quantum Mechanics in One Dimension”. John Hopkins, Baltimore.

[25]. Jenks, S.E. 2012. “Selecting Semiconductor Materials for the Quantum Dot Intermediate Band Solar Cell”. Drexel University.

[26]. Marti, A., Cuadra, L., Luque, A. 2000. “Quantum dot intermediate band solar cell,” IEEE Photovolt. Special. Conf., 940–943.

[27]. Aroutiounian, V., Petrosyan, S., Khachatryan, A., Touryan. K. 2001.” Quantum Dot Solar Cells”. Yerevan State University, 1Manoukian St., Yerevan 375049, Armenia, USA.

[28]. Masetti, G., Severi, M., Solmi, S. 1983. “Modeling of Carrier Mobility Against Carrier Concentration in Arsenic, Phosphorous and Boron doped Silicon”. IEEE Trans. Elec. Dev. ED-30: pp. 764-769

[29] Murray, C. B., Norris, D. J., Bawendi, M. G. 1993. "Synthesis and characterization of nearly monodisperse CdE (E = sulfur, selenium, tellurium) semiconductor nanocrystallites". Journal of the American Chemical Society 115 (19): 8706. doi:10.1021/ja00072a025

[30]. Vurgaftman, I., Meyer, Band., J.R. 2001. “parametersfor III–V compound semiconductors and their alloys”. J. Appl. Phys. 89, pp. 5815–62.

[31]. Shockley, W., Queisser, H. J. 1961. J. Appl. Phys., 32, 510.

[32]. Yi-Hsien Lin and Jean-Fu Kiang,"Efficiency Improvement of p-i-n Solar Cell by Embedding Quantum Dots". 2014. *Progress In Electromagnetics Research*, Vol. 146, 167–180.

[33]. Wiemer, M., Sabin's, V., Yuen, H. 2011. "Proc. of SPIE", 8108, 810804.

[34]. Gerald, S., Carsten, B., Andreas, W.B. 2010. "External Quantum Efficiency Measurements of Germanium Bottom Sub cells: Measurements Artifacts and Correction Procedures".IEEE, European Space Agency, ESTEC, Keplerlaan, 2200AG Noordwijk, the Netherlands