THESIS PAPER

ON

"SIMULATION OF A 2D P-N JUNCTION IN SILICON THIN FILM INCORPORATING QUANTUM TRANSPORT FOR CARRIERS"

Submitted by

Munna Kumar Basak	Md. Al-Amin Joarder
ID. NO: 112-33-576	ID. NO: 112-33-664
Dept. of EEE	Dept. of EEE
Daffodil International University	Daffodil International University

Supervised by

Md. Mahmudur Rahman

Senior Lecturer

Department of Electrical & Electronic Engineering (EEE)

Daffodil International University

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APPROVAL

This Thesis Titled **"SIMULATION OF A 2D P-N JUNCTION IN SILICON THIN FILM INCORPORATING QUANTUM TRANSPORT FOR CARRIERS"** submitted by **Munna Kumar Basak** and **Md. Al-Amin Joarder** to the Department of Electrical and Electronic Engineering, Daffodil International University, has been accepted as satisfactory for the partial fulfillment of the requirement for the degree of B.Sc. in Electrical and Electronic Engineering and approved as to its style and contents. The presentation has been held on **27 August, 2015**.

BOARD OF EXAMINERS

Professor Dr.M.Shamsul Alam
Dean
Faculty of Engineering   **Chairman**
Daffodil International University

Dr.Md.Fayzur Rahman   **Internal Examiner**
Professor And Head
Department of EEE
Faculty of Engineering
Daffodil International University

DECLARATION

We hereby declare that, this thesis has been done by us under the supervision of **Md. Mahmudur Rahman, Lecturer,** EEE, Daffodil International University We also declare that neither this thesis nor any part of this project has been submitted elsewhere for award of any degree or diploma.

Supervised by:

Md. Mahmudur Rahman   **Signature   :**
Department of EEE   **Date   :**
Faculty of Engineering
Daffodil International University

Submitted by:

Munna Kumar Basak
ID No: 112-33-576
Department of EEE
Faculty of Engineering
Daffodil International University

MD. Al-Amin Joarder
ID No: 112-33-664
Department of EEE
Faculty of Engineering
Daffodil International University

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ABSTRACT

Silicon nanostructures have recently been a subject of interest demonstrating optical properties like luminescence. The Scientific community predicts quantum effects to be the predominant cause for such optical properties of silicon nanostructures. With this view as a motive, a simulation model of a 2D thin film quantum confined 2D p-n junction in silicon is developed in this work.

A thin film silicon layer is considered in the regime of strong confinement. A p-n junction in such a film is considered so that the carriers are confined in thickness dimension while they are quantum mechanically transported along the device length. The transverse dimension in considered infinitely wide for plane wave approximation. For device simulation, after a careful study of various schemes to incorporate quantum effects, it was decided to use self-consistent Schrodinger-Poisson method.

The simulation is done in MATLAB. For solution, instead of winger function or Green's function, a more direct wave-function perspective is taken. First the equilibrium condition was simulated and then extension under externally applied voltage was carried out.

CONTENTS

LIST OF FIGURES

LIST OF ABBREVATION

2-DEG : Tow Dimensional Electron Gas

SOI : Silicon On Insulator

IC : Integrated Circuit

3D : Three Dimension

2D : Two Dimension

1D : One Dimension

PL : Photoluminescence

EL : Electroluminescence

PS : Porous Silicon

eV : Electron Volt

meV : Milli-Electron Volt

DG : Density Gradient

QHD : Quantum Hydro Dynamic

NEGF : Non-Equilibrium Green's Function

SP : Schrodinger-Poisson

SCF : self Consistent Field

DOS : Density Of States

FEM : Finite Element Method

MOS : Metal Oxide Semiconductor

LIST OF SYMBOLS

Symbol	Parameter
J	Current density
Q	Electronic charge
μ	Mobility
k_B	Boltzmann constant
n	Electron density
p	Charge density
m	Mass of particle
U,V	System potential
π	Pi
γ	Source term
δ	Dirac delta
ε	Dielectric Constant
λ	Wave length
v	Frequency
ψ	Wave function
Γ	Broadening matrix
$\sum$	Self energy matrix
Φ	Basis function
φ	Expansion coefficient
T	Temperature
E_g	Band gap energy
E_f	Fermi energy
E_c	Conduction band edge
E_v	Valance band edge

N_d, N_a Doping concentration

f_{FD} Fermi-Dirac distribution

$F_{-1/2}$ Fermi integral

$g(E)$ Density of states

E_m Sub-band energy

$\hbar$ Reduced Plank's constant

G   Green's function

I   Identity matrix

H   Hamiltonian matrix

K   Wave vector

Introduction

Optical and optoelectronic properties of silicon nanostructures have recently been a subject of interest. Though bulk silicon is an indirect semiconductor and generally unsuitable for optoelectronic devices. Structures such as porous silicon or quantum dots have been reported to emit light. Some research has been done with lateral junctions in quantum wells which demonstrates high-frequency operation and is suggestive of the possibility of light generation. Hence instead of approximate analytical model, constructing a simulation model and exploring the possibility of direct recombination for such devices in silicon is in order.

1.1.   Objective:

The primary objective of this work is to investigate a thin film silicon p-n junction incorporating quantum effects. As the thickness of the thin is reduced, it essentially becomes a quantum device with 2D electron gas (2=DEG) having 1D confinement, and a quantum mechanical approach becomes necessary to model such device. Models with approximate analysis are only suggestive of features of such devices, so a numerical simulation model becomes necessary for a more comprehensive insight. Hence, a simulation model is constructed for such a device. Due to the requirement of unfeasibly huge computational resource required in direct discretized approach for a 2D device. It becomes prudent to such a device, in this wore decoupled set of 1D equation is applied to the 2D bipolar system.

1.2.   Motivation

Recently conducted studies have resulted in the anticipation that a silicon nanostructure might be a sustainable source of light. But with simple nanostructures it is yet hard to achieve reproducibility and the search for a nanodevice in silicon for light emission is on the way. In this regard, a thorough analysis of such reduced dimensional device is sought for. Thin films of silicon are now possible on silicon on insulator (SOI) structure, and if thickness is reduced below

5nm then quantum confinement occur in that direction and this may pave the way towards silicon optoelectronic.

Reporting of simulation results of lateral p-n junction in quantum well in silicon is rare. Analytic studies on other material do indicate high-frequency operator of such a device. Other studies suggest that quantum effects could be the origin behind electroluminescence and light emission from silicon nanostructures. So a comprehensive simulation of a lateral p-n junction in silicon quantum well could help find a sustainable silicon light emitting structure.

1.3.   Application

Most of the SOI structures are now being used for bipolar devices. But for photonics it becomes important to use a bipolar device for recombination of holes and electrons. In that regard, a thin film silicon p-n junction could offer a new possibility. Silicon light emitting device could find two very important uses:

1. Optical and electronic circuit integration to achieve integrated optoelectronics, which now in impossible as compound semiconductor alloys are used for optoelectronics.
2. Optical interconnect could replace slow electric interconnects, which remain a bottleneck towards high=speed integrated chips, which for a long time to come will continue to be fabricated in silicon.

CHAPTER-02

Literature review

2.1 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 voltage applied 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-charged electrons, 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.

Elemental semiconductors include antimony, arsenic, boron, carbon, germanium, selenium, silicon, sulfur, and tellurium. Silicon is the best-known of these, forming the basis of most integrated circuits (ICs).

2.1.1 Characteristics of silicon:

Physical:

Silicon is a solid at room temperature, with relatively high melting and boiling points of 1414 and 3265 °C, respectively. Like water, it has a greater density in a liquid state than in a solid state, and so, like water but unlike most substances, it does not contract when it freezes, but expands. With a relatively high thermal conductivity of 149 $W \cdot m^{-1} \cdot K^{-1}$, silicon conducts heat well [1].

3
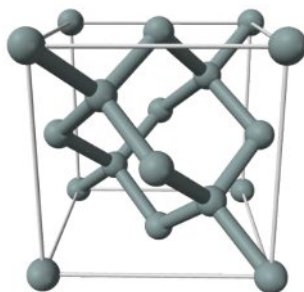
Figure 2.1: Silicon crystallizes in a diamond cubic crystal structure

Chemical:

Silicon is a metalloid, readily either donating or sharing its four outer electrons and it typically forms four bonds. Like carbon, its four bonding electrons give it opportunities to combine with many other elements or compounds to form a wide range of compounds. Unlike carbon, it can accept additional electrons and form five or six bonds in a sometimes more labilesilicate form. Tetra-valent silicon is relatively inert, but still reacts with halogens and dilute alkalis, but most acids (except for some hyper-reactive combinations of nitric acid and hydrofluoric acid) have no known effect on it.

Figure 2.1.2: Silicon powder

Isotopes:

Naturally occurring silicon is composed of three stable isotopes, silicon-28, silicon-29, and silicon-30, with silicon-28 being the most abundant (92% natural abundance).[14] Out of these, only silicon-29 is of use in NMR and EPR spectroscopy.[15] Twenty radioisotopes have been characterized, with the most stable being silicon-32 with a half-life of 170 years, and silicon-31 with a half-life of 157.3 minutes [2].

2.2: Direct and indirect band gaps:

In semiconductor physics, the band gap of a semiconductor is always one of two types, a direct band gap or an indirect band gap. The minimal-energy state in the conduction band and the maximal-energy state in the valence band are each characterized by a certain crystal momentum (k-vector) in the Brillion zone. If the k-vectors are the same, it is called a "direct gap". If they are different, it is called an "indirect gap". The band gap is called "direct" if the momentum of electrons and holes is the same in both the conduction band and the valence band; an electron can directly emit a photon. In an "indirect" gap, a photon cannot be emitted because the electron must pass through an intermediate state and transfer momentum to the crystal lattice.

Indirect Band Gap

Energy

Conduction Band

Phonon assisted transition

Valence Band
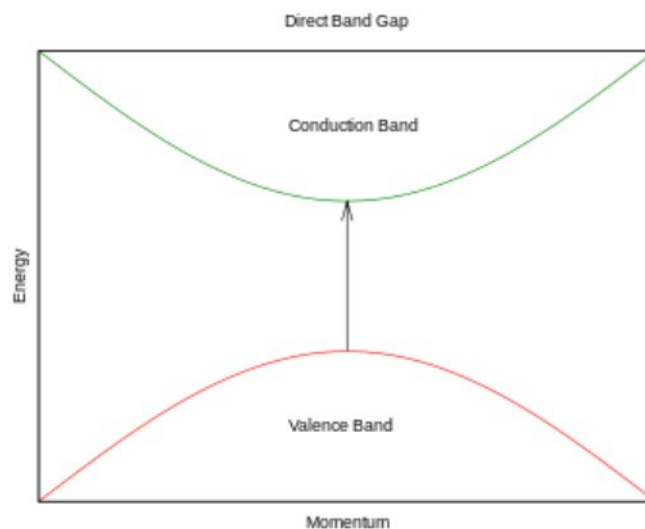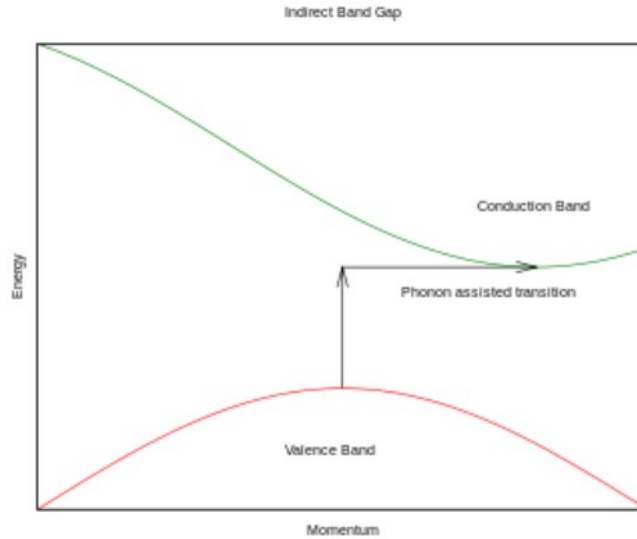
Momentum

Figure 2.2: Energy vs. crystal momentum for a semiconductor with an indirect band gap.

2.3 Doping:

Doping is the process of adding impurities to intrinsic **semiconductors** to alter their properties. Normally Trivalent and Pentavalent elements are used to dope Silicon and Germanium. When a intrinsic **semiconductor** is **doped** with trivalent impurity it becomes a P-Type **semiconductors**. When a intrinsic **semiconductor** is **doped** with Pentavalent impurity it becomes a N-Type **semiconductors.**
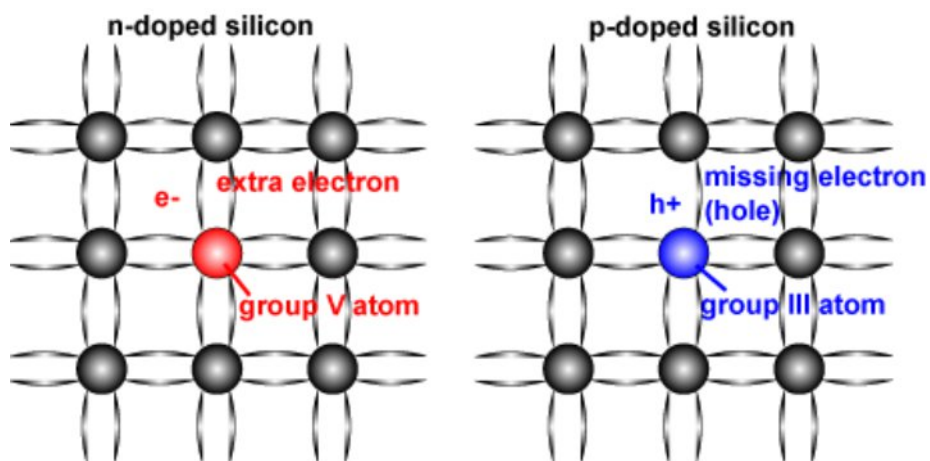
Figure 2.3: N-Type and P-Type doped silicon.

6

2.4.   How Doping Works:

Atoms follow a rule called Octet Rule. According to Octet-rule atoms are stable when there are eight electrons in their valence. If not atoms readily accept or share neighboring atoms to achieve eight electrons in their valance shell. In the silicon lattice each silicon atom is surrounded by four silicon atoms. Each silicon atom share one of its electron in the valance shell to its neighbor to satisfy the octet-rule. A schematic diagram of an intrinsic semiconductor is shown in image right (Figure: Intrinsic Silicon Lattice).

Now let's see what will happen when we pop in a pentavalent element into the lattice. As you can see the image (Figure: N-type), we have doped the silicon lattice with Phosphorous, a pentavalent element. Now pentavalent element has five electrons, so it shares a electron with each of the four neighboring silicon atoms, hence four atoms are tied up with the silicon atoms in the lattice. This leaves an electron extra. This excess electron is free to move and is responsible conduction. Hence N-type (Negative Type) extrinsic semiconductor (silicon in this case) is made by doping the semiconductor with pentavalent element.

To create a P-type semiconductor, all we must do is to pop in a trivalent element into the lattice. A trivalent element has three electrons in its valence shell. It shares three electrons with three neighboring silicon atoms in the lattice, the fourth silicon atom demands an electron but the trivalent atom has no more electrons to share. This creates a void in lattice which we call it has hole. Since the electron is deficient, the hole readily accepts an electron; this makes it a P-type (Positive type) extrinsic semiconductor.

As you can see at image (Figure: P-type), we have popped in boron (trivalent element) in silicon lattice. This has created a hole making the semiconductor a P-type material.

The case is no different in Germanium. Its behaves same as silicon however some properties do differ which makes germanium based devices used in certain application and silicon based devices used in other applications.

7

2.5.   P-Type & N-Type Semiconductors: [3]

P-type:

In a pure (intrinsic) Si or Ge semiconductor, each nucleus uses its four valence electrons to form four covalent bonds with its neighbors (see figure below). Each ionic core, consisting of the nucleus and non-valent electrons, has a net charge of +4, and is surrounded by 4 valence electrons. Since there are no excess electrons or holes In this case, the number of electrons and holes present at any given time will always be equal.
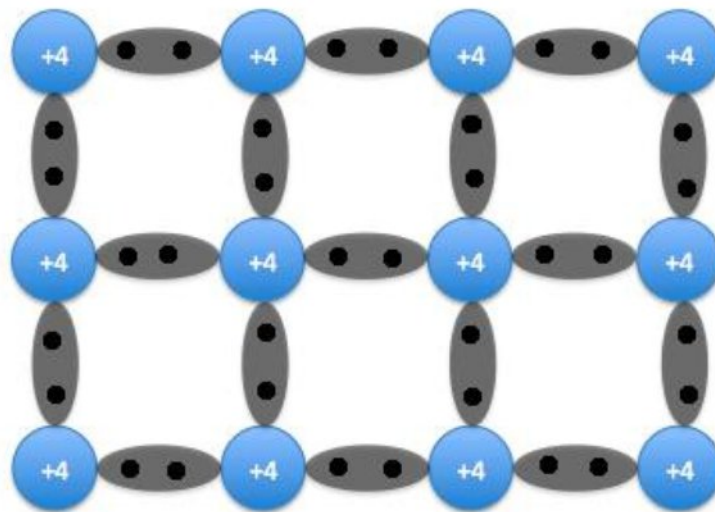
Figure 2.5.1: An intrinsic semiconductor. Note each +4 ion is surrounded by four electrons.

Now, if one of the atoms in the semiconductor lattice is replaced by an element with three valence electrons, such as a Group 3 element like Boron (B) or Gallium (Ga), the electron-hole balance will be changed. This impurity will only be able to contribute three valence electrons to the lattice, therefore leaving one excess hole (see figure below). Since holes will "accept" free electrons, a Group 3 impurity is also called an acceptor.
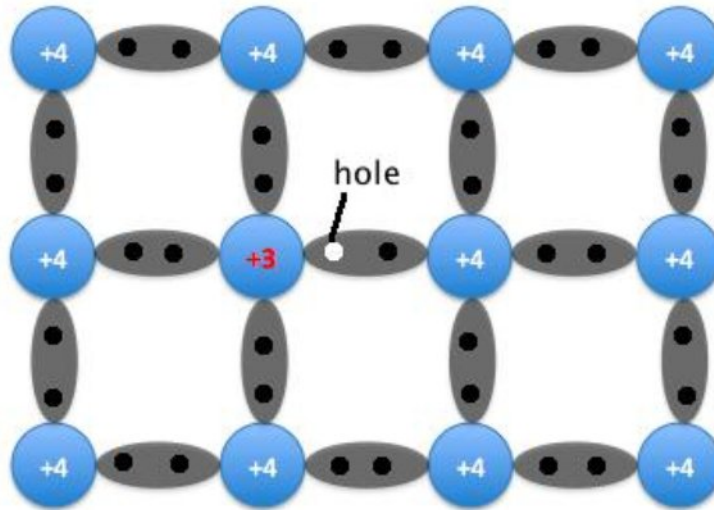
Figure 2.5.2: A semiconductor doped with an acceptor. An excess hole is now present.

Because an acceptor donates excess holes, which are considered to be positively charged, a semiconductor that has been doped with an acceptor is called a p-type semiconductor; "p" stands for positive. Notice that the material as a whole remains electrically neutral. In a p-type semiconductor, current is largely carried by the holes, which outnumber the free electrons. In this case, the holes are the majority carriers, while the electrons are the minority carriers.

N-type:

In addition to replacing one of the lattice atoms with a Group 3 atom, we can also replace it by an atom with five valence electrons, such as the Group 5 atoms arsenic (As) or phosphorus (P). In this case, the impurity adds five valence electrons to the lattice where it can only hold four. This means that there is now one excess electron in the lattice (see figure below). Because it donates an electron, a Group 5 impurity is called a donor. Note that the material remains electrically neutral.
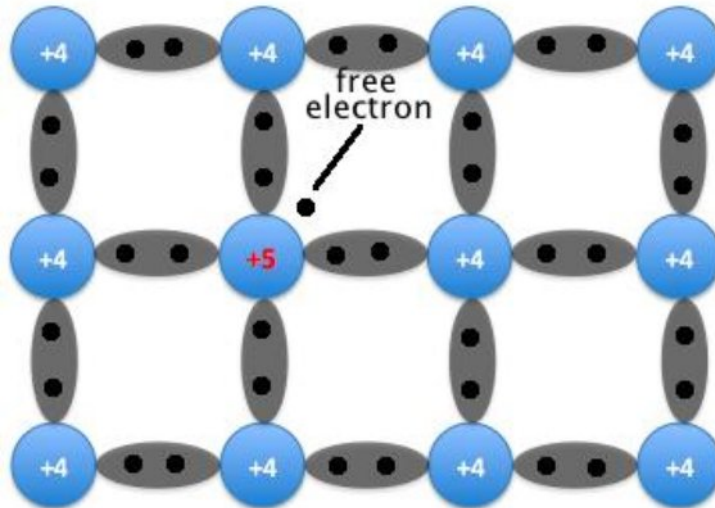
Figure 2.5.3: A semiconductor doped with a donor. A free electron is now present.

Donor impurities donate negatively charged electrons to the lattice, so a semiconductor that has been doped with a donor is called an n-type semiconductor; "n" stands for negative. Free electrons outnumber holes in an n-type material, so the electrons are the majority carriers and holes are the minority carriers.

2.6. P-N Junction:

P-n junctions are formed by joining n-type and p-type semiconductor materials, as shown below. Since the n-type region has a high electron concentration and the p-type a high hole concentration, electrons diffuse from the n-type side to the p-type side.

In other world, if we join (or fuse) these two Semiconductor Materials together they behave in a very different way merging together and producing what is generally known as a "**PN Junction**".

When the N-type semiconductor and P-type semiconductor materials are first joined together a very large density gradient exists between both sides of the PN junction. The result is that some of the free electrons from the donor impurity atoms begin to migrate across this newly formed junction to fill up the holes in the P-type material producing negative ions. However, because the electrons have moved across the PN junction from the N-type silicon to the P-type silicon, they leave behind positively charged donor ions (N_D) on the negative side and now the holes from

10

the acceptor impurity migrate across the junction in the opposite direction into the region where there are large numbers of free electrons.

As a result, the charge density of the P-type along the junction is filled with negatively charged acceptor ions (N_A), and the charge density of the N-type along the junction becomes positive. This charge transfer of electrons and holes across the PN junction is known as diffusion. The width of these P and N layers depends on how heavily each side is doped with acceptor density N_A, and donor density N_D, respectively.

This process continues back and forth until the number of electrons which have crossed the junction
have a large enough electrical charge to repel or prevent any more charge carriers from crossing over the junction. Eventually a state of equilibrium (electrically neutral situation) will occur producing a "potential barrier" zone around the area of the junction as the donor atoms repel the holes and the acceptor atoms repel the electrons.

Since no free charge carriers can rest in a position where there is a potential barrier, the regions on either sides of the junction now become completely depleted of any more free carriers in comparison to the N and P type materials further away from the junction. This area around the **PN Junction** is now called the Depletion Layer.
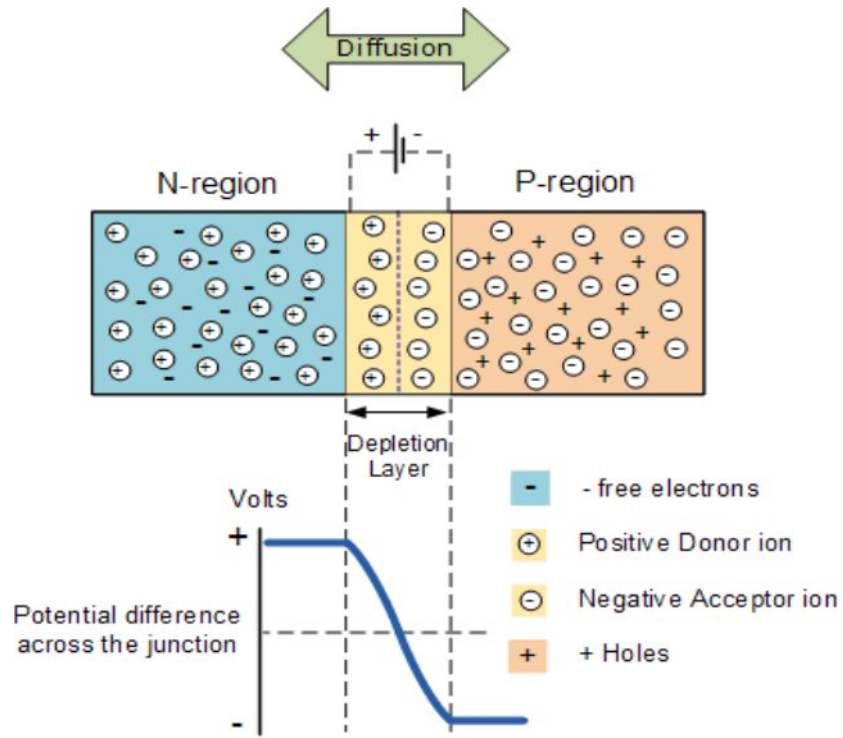
Figure 2.6: P-N junction

The total charge on each side of a *PN Junction* must be equal and opposite to maintain a neutral charge condition around the junction. If the depletion layer region has a distance D, it therefore must therefore penetrate into the silicon by a distance of Dp for the positive side, and a distance of Dn for the negative side giving a relationship between the two of $Dp.N_A = Dn.N_D$ in order to maintain charge neutrality also called equilibrium.

2.7. P-N Junction Distance:
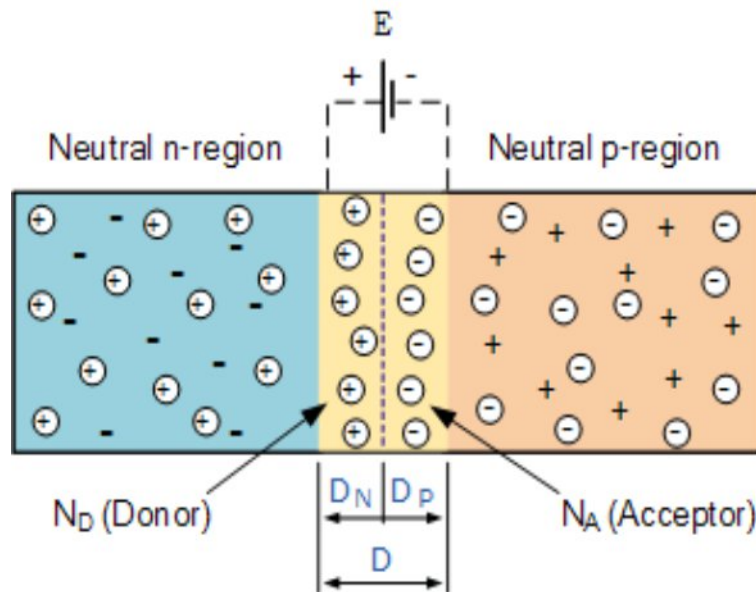
As the N-type material has lost electrons and the P-type has lost holes, the N-type material has become positive with respect to the P-type. Then the presences of impurity ions on both sides of the junction cause an electric field to be established across this region with the N-side at a positive voltage relative to the P-side. The problem now is that a free charge requires some extra energy to overcome the barrier that now exists for it to be able to cross the depletion region junction.

This electric field created by the diffusion process has created a "built-in potential difference" across the junction with an open-circuit (zero bias) potential of

$$E_o = V_T \ln\left(\frac{N_D . N_A}{n_i^2}\right)$$

Where: E_o is the zero bias junction voltage, V_T the thermal voltage of 26mV at room temperature, N_D and N_A are the impurity concentrations and n_i is the intrinsic concentration.

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2.8. Junction Diode Symbol and Static I-V Characteristics. [4]
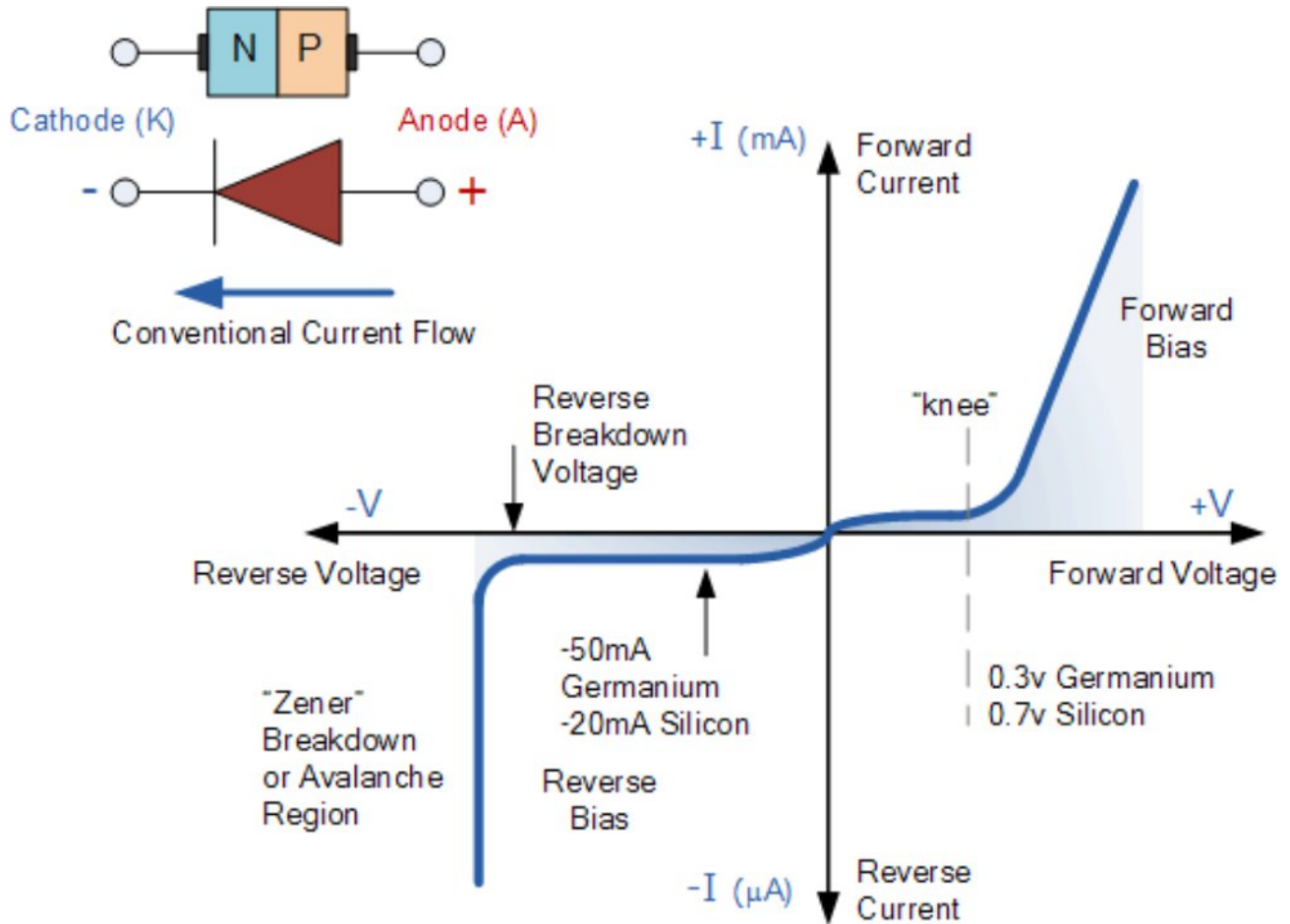
Figure 2.8: I-V Characteristics

But before we can use the PN junction as a practical device or as a rectifying device we need to firstly **bias** the junction, ie connect a voltage potential across it. On the voltage axis above, "Reverse Bias" refers to an external voltage potential which increases the potential barrier. External voltages which decrease the potential barrier is said to act in the "Forward Bias" direction.

There are two operating regions and three possible "biasing" conditions for the standard **Junction Diode** and these are:

- 1.Zero Bias – No external voltage potential is applied to the PN junction diode

14

- 2. Reverse Bias – The voltage potential is connected negative, (-ve) to the P-type material and positive, (+ve) to the N-type material across the diode which has the effect of **Increasing** the PN junction diode's width.
- 3. Forward Bias – The voltage potential is connected positive, (+ve) to the P-type material and negative, (-ve) to the N-type material across the diode which has the effect of **Decreasing** the PN junction diodes width.

2.9. Zero Biased Junction Diode:

When a diode is connected in a **Zero Bias** condition, no external potential energy is applied to the PN junction. However if the diodes terminals are shorted together, a few holes (majority carriers) in the P-type material with enough energy to overcome the potential barrier will move across the junction against this barrier potential. This is known as the "**Forward Current**" and is referenced as I_F

Likewise, holes generated in the N-type material (minority carriers), find this situation favorable and move across the junction in the opposite direction. This is known as the "**Reverse Current**" and is referenced as I_R. This transfer of electrons and holes back and forth across the PN junction is known as diffusion, as shown below.
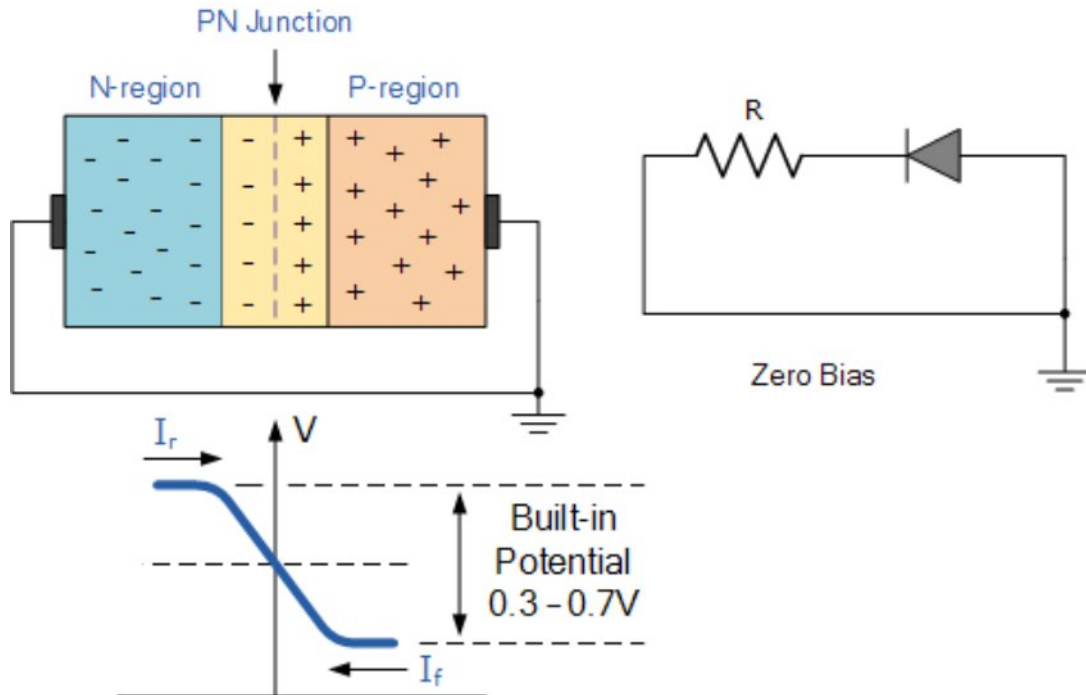
Figure 2.9: Zero Biased PN Junction Diode

The potential barrier that now exists discourages the diffusion of any more majority carriers across the junction. However, the potential barrier helps minority carriers (few free electrons in the P-region and few holes in the N-region) to drift across the junction.

Then an "Equilibrium" or balance will be established when the majority carriers are equal and both moving in opposite directions, so that the net result is zero current flowing in the circuit. When this occurs the junction is said to be in a state of "**Dynamic Equilibrium**".

The minority carriers are constantly generated due to thermal energy so this state of equilibrium can be broken by raising the temperature of the PN junction causing an increase in the generation of minority carriers, thereby resulting in an increase in leakage current but an electric current cannot flow since no circuit has been connected to the PN junction.

2.10.1. Reverse Biased PN Junction Diode:

When a diode is connected in a **Reverse Bias** condition, a positive voltage is applied to the N-type material and a negative voltage is applied to the P-type material.

The positive voltage applied to the N-type material attracts electrons towards the positive electrode and away from the junction, while the holes in the P-type end are also attracted away from the junction towards the negative electrode.

The net result is that the depletion layer grows wider due to a lack of electrons and holes and presents a high impedance path, almost an insulator. The result is that a high potential barrier is created thus preventing current from flowing through the semiconductor material.

Increase in the Depletion Layer due to Reverse Bias:
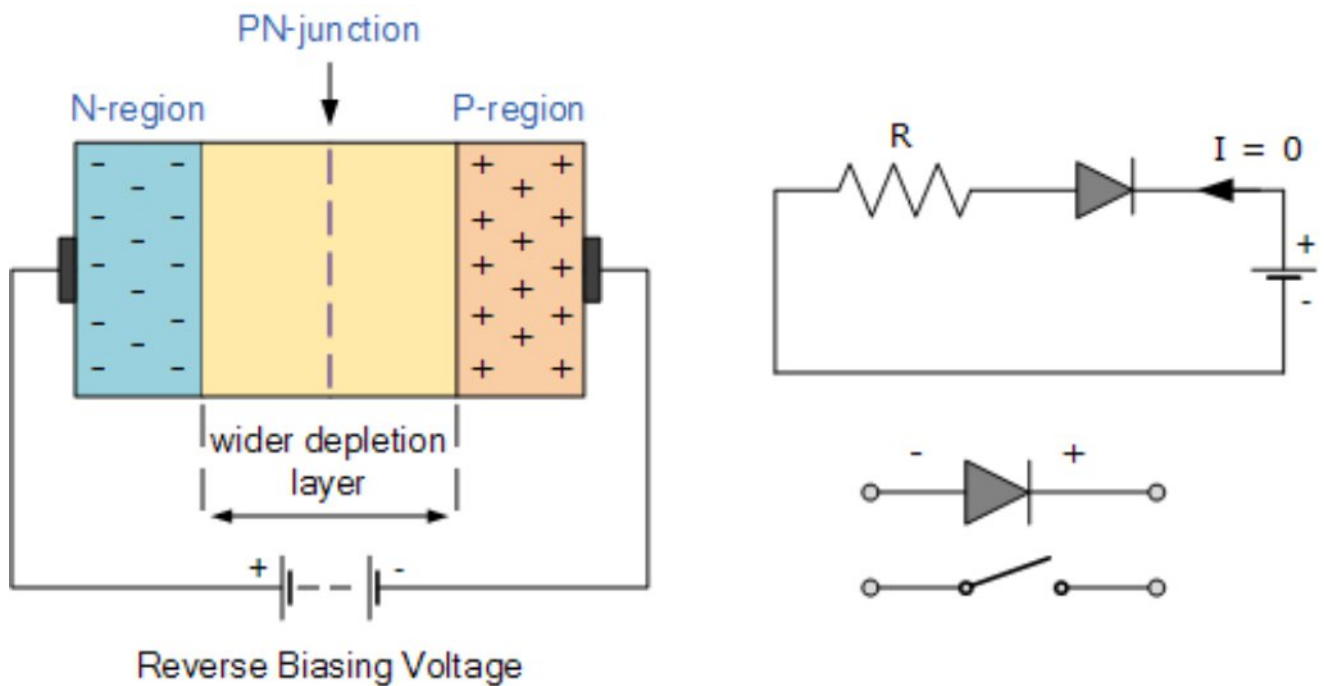
Figure 2.10.1: Reverse Bias

This condition represents a high resistance value to the PN junction and practically zero current flows through the junction diode with an increase in bias voltage. However, a very small **leakage current** does flow through the junction which can be measured in micro-amperes, (µA).

One final point, if the reverse bias voltage Vr applied to the diode is increased to a sufficiently high enough value, it will cause the diode's PN junction to overheat and fail due to the avalanche effect around the junction. This may cause the diode to become shorted and will result in the flow of maximum circuit current and this shown as a step downward slope in the reverse static characteristics curve below.

Reverse Characteristics Curve for a Junction Diode:
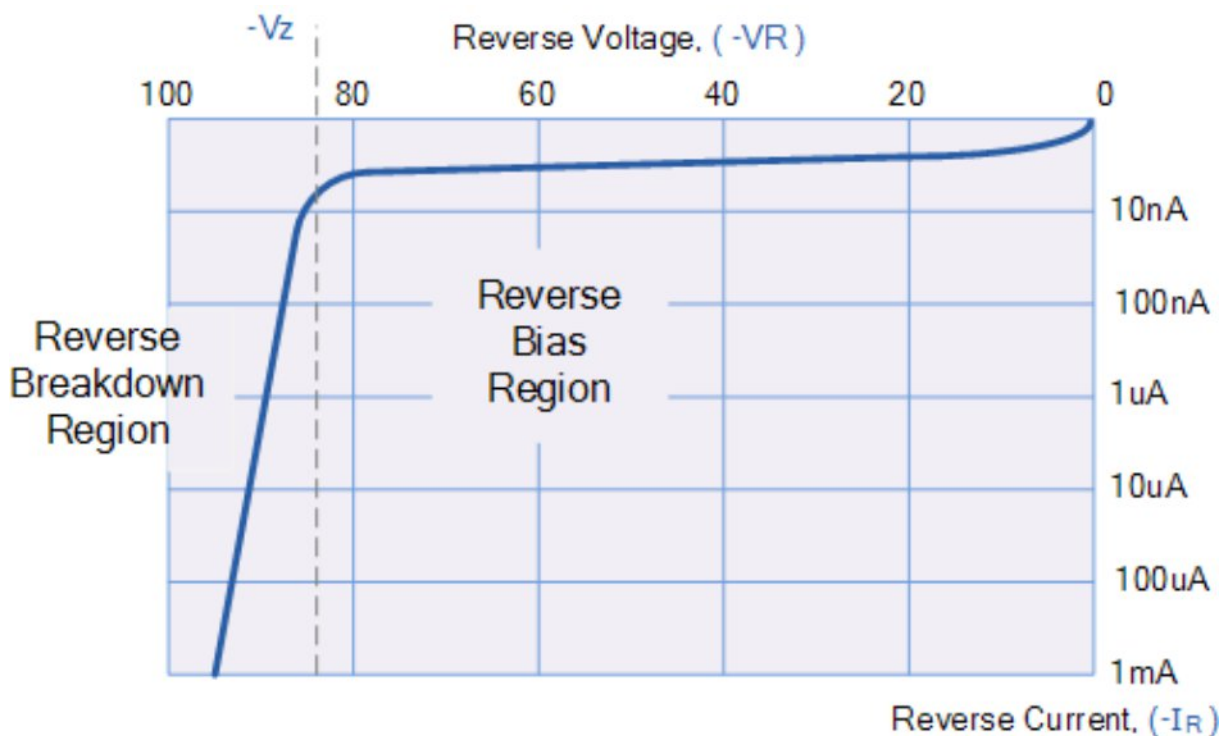
Sometimes this avalanche effect has practical applications in voltage stabilising circuits where a series limiting resistor is used with the diode to limit this reverse breakdown current to a preset maximum value thereby producing a fixed voltage output across the diode. These types of diodes are commonly known as Zener Diodes and are discussed in a later tutorial.

2.10.2. Forward Biased PN Junction Diode:

When a diode is connected in a **Forward Bias** condition, a negative voltage is applied to the N-type material and a positive voltage is applied to the P-type material. If this external voltage becomes greater than the value of the potential barrier, approx. 0.7 volts for silicon and 0.3 volts for germanium, the potential barriers opposition will be overcome and current will start to flow.

This is because the negative voltage pushes or repels electrons towards the junction giving them the energy to cross over and combine with the holes being pushed in the opposite direction towards the junction by the positive voltage. This results in a characteristics curve of zero current flowing up to this voltage point, called the "knee" on the static curves and then a high current flow through the diode with little increase in the external voltage as shown below.

Forward Characteristics Curve for a Junction Diode
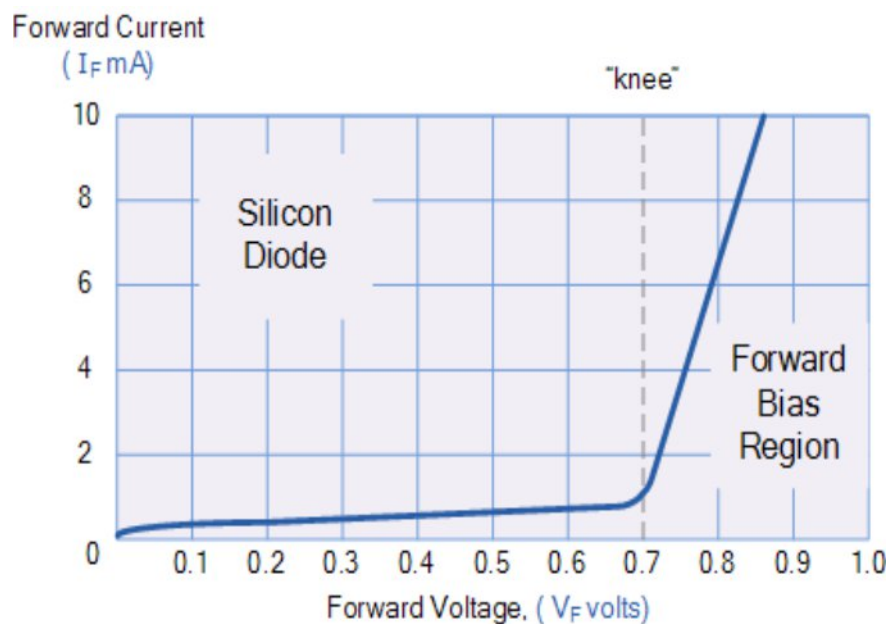
Figure 2.10.2: Forward Characteristics Curve for a Junction Diode

The application of a forward biasing voltage on the junction diode results in the depletion layer becoming very thin and narrow which represents a low impedance path through the junction thereby allowing high currents to flow. The point at which this sudden increase in current takes place is represented on the static I-V characteristics curve above as the "knee" point.

Reduction in the Depletion Layer due to Forward Bias
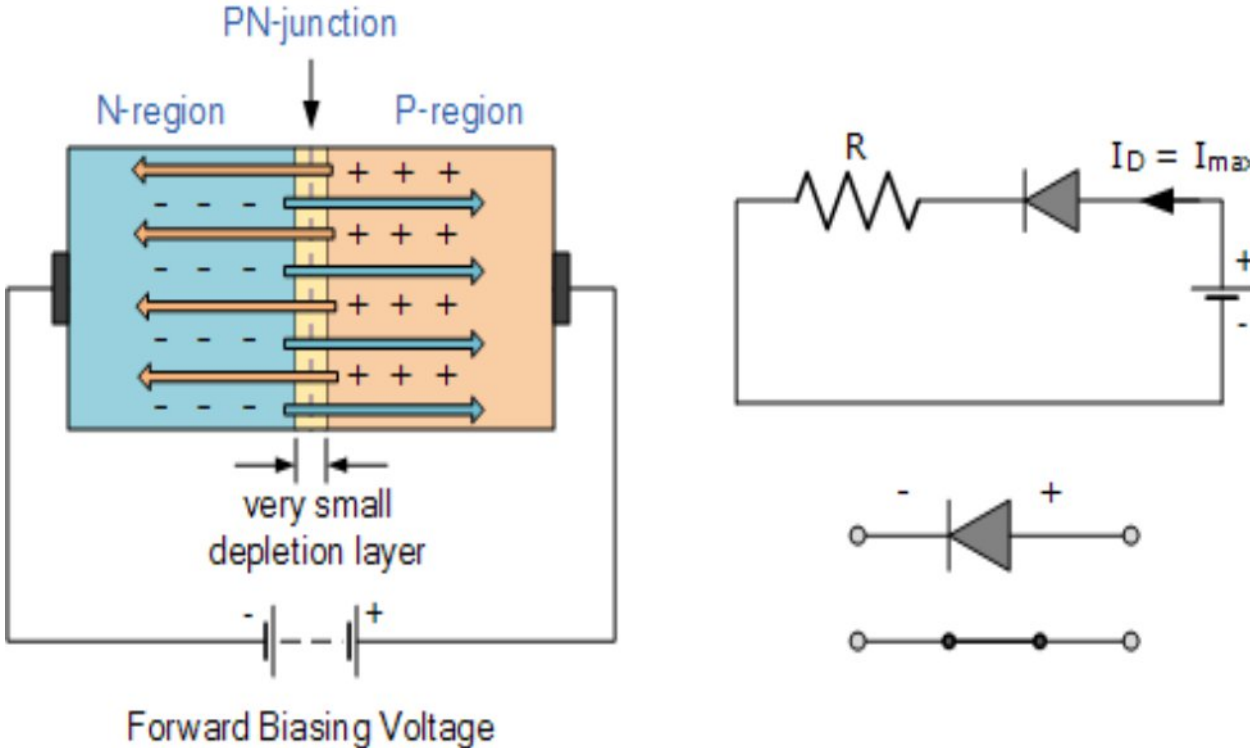
This condition represents the low resistance path through the PN junction allowing very large currents to flow through the diode with only a small increase in bias voltage. The actual potential difference across the junction or diode is kept constant by the action of the depletion layer at approximately 0.3v for germanium and approximately 0.7v for silicon junction diodes.

Since the diode can conduct "infinite" current above this knee point as it effectively becomes a short circuit, therefore resistors are used in series with the diode to limit its current flow. Exceeding its maximum forward current specification causes the device to dissipate more power in the form of heat than it was designed for resulting in a very quick failure of the device.

2.11. Junction Diode Summary:

The PN junction region of a **Junction Diode** has the following important characteristics:

- Semiconductors contain two types of mobile charge carriers, **Holes** and **Electrons**.
- The holes are positively charged while the electrons negatively charged.
- A semiconductor may be doped with donor impurities such as Antimony (N-type doping), so that it contains mobile charges which are primarily electrons.
- A semiconductor may be doped with acceptor impurities such as Boron (P-type doping), so that it contains mobile charges which are mainly holes.
- The junction region itself has no charge carriers and is known as the depletion region.
- The junction (depletion) region has a physical thickness that varies with the applied voltage.
- When a diode is **Zero Biased** no external energy source is applied and a natural **Potential Barrier** is developed across a depletion layer which is approximately 0.5 to 0.7v for silicon diodes and approximately 0.3 of a volt for germanium diodes.
- When a junction diode is **Forward Biased** the thickness of the depletion region reduces and the diode acts like a short circuit allowing full current to flow.
- When a junction diode is **Reverse Biased** the thickness of the depletion region increases and the diode acts like an open circuit blocking any current flow, (only a very small leakage current).

We have also seen above that the diode is two terminal non-linear device whose I-V characteristic are polarity dependent as depending upon the polarity of the applied voltage, V_D the diode is either *Forward Biased*, $V_D > 0$ or *Reverse Biased*, $V_D < 0$. Either way we can model these current-voltage characteristics for both an ideal diode and for a real diode.

Quantum Mechanics for Nanodevices

The purely mathematical postulations that make quantum mechanics the tool for actually describing nature is too intricate and exceed the scope of this report. The more used Schrodinger's version of the mechanics is adopted as it gives a better insight to the subject, and provides for the practical means of modeling a nanodevice.

3.1. Translate the Schrödinger Equation to Three Dimensions:

In quantum physics, you can break the three-dimensional Schrödinger equation into three one-dimensional Schrödinger equations to make it easier to solve 3D problems. In one dimension, the time-dependent Schrödinger equation (which lets you find a wave function) looks like this:

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)+V(x,t)\psi(x,t)=i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

And you can generalize that into three dimensions like this:

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z,t)+V(r)\psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\psi(x,y,z,t)$$

Using the Laplacian operator, you can recast this into a more compact form. Here's what the Laplacian looks like:

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)=\nabla^2$$

And here's the 3D Schrödinger equation using the Laplacian:

$$\frac{-\hbar^2}{2m}\nabla^2\psi(x,y,z,t)+V(x,y,z,t)\psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\psi(x,y,z,t)$$

To solve this equation, when the potential doesn't vary with time, break out the time-dependent part of the wave function:

$$\psi(x,y,z,t) = \psi(x,y,z)e^{-iEt/\hbar}$$

Here,

$$\psi(x,y,z)$$

is the solution of the time-independent Schrödinger equation, and E is the energy:

$$\frac{-\hbar^2}{2m}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

So far, so good. But now you've run into a wall — the expression

$$\nabla^2\psi(x,y,z)$$

is in general very hard to deal with, so the current equation is in general very hard to solve.

So what should you do? Well, you can focus on the case in which the equation is separable — that is, where you can separate out the x, y, and z dependence and find the solution in each dimension separately. In other words, in separable cases, the potential, V(x, y, z), is actually the sum of the x, y, and z potentials:

V(x, y, z) = $V_x(x)$ + $V_y(y)$ + $V_z(z)$

Now you can break the Hamiltonian in

$$\frac{-\hbar^2}{2m}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$$

into three Hamilitonians, H_x, H_y, and H_z:

$$\left(H_x + H_y + H_z\right)\psi(x,y,z) = E\psi(x,y,z)$$

23

Where,

- $H_x = \dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V_x(x)$

- $H_y = \dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial y^2} + V_y(y)$

- $H_z = \dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial z^2} + V_z(z)$

When you divide up the Hamiltonian as in

$$\left(H_x + H_y + H_z\right)\psi(x,y,z) = E\psi(x,y,z),$$

you can also divide up the wave function that solves that equation. In particular, you can break the wave function into three parts, one for x, y, and z:

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

Where X(x), Y(y), and Z(z) are functions of the coordinates x, y, and z and are not to be confused with the position operators. This separation of the wave function into three parts is going to make life considerably easier, because now you can break the Hamiltonian up into three separate operators added together:

$$\left(\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V_x(x)\right) + \left(\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial y^2} + V_y(y)\right) + \left(\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial z^2} + V_z(z)\right) = H$$

$E = E_x + E_y + E_z$

So you now have three independent Schrödinger equations for the three dimensions:

24

- $\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}X(x)+V(x)X(x)=E_x\,X(x)$

- $\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial y^2}Y(y)+V(y)Y(y)=E_y\,Y(y)$

- $\dfrac{-\hbar^2}{2m}\dfrac{\partial^2}{\partial z^2}Z(z)+V(z)Z(z)=E_z\,Z(z)$

This system of independent differential equations looks a lot easier to solve than

$$\left(H_x+H_y+H_z\right)\psi(x,y,z)=E\psi(x,y,z).$$

In essence, you've broken the three-dimensional Schrödinger equation into three one-dimensional Schrödinger equations. That makes solving 3D problems tractable.

3.2.   Poisson's equation:

In mathematics, **Poisson's equation** is a partial differential equation of elliptic type with broad utility in electrostatics, mechanical engineering and theoretical physics. It is used, for instance, to describe the potential energy field caused by a given charge or mass density distribution. The equation is named after the Frenchmathematician, geometer, and physicistSiméon Denis Poisson.

Statement of the equation

Poisson's equation is

$$\Delta\varphi = f$$

where $\Delta$is the Laplace operator, and f and φ are real or complex-valued functions on a manifold. Usually, f is given and φ is sought. When the manifold is Euclidean space, the Laplace operator is often denoted as $\nabla^2$and so Poisson's equation is frequently written as

$$\nabla^2\varphi = f.$$

In three-dimensional Cartesian coordinates, it takes the form

25

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z) = f(x,y,z).$$

When $= 0$ we retrieve Laplace's equation.

Poisson's equation may be solved using a Green's function.

3.3. Models of quantum devices:

- The density gradient (DG) method
- Quantum hydro-dynamic model (QHD)
- Van Dort model
- Self-consistent Schrodinger-Poisson model
- Non equilibrium Greens Function (NEGF) formalism

3.4. Self-consistent Schrodinger-Poisson model:

This model is more accurate model of the actual quantum mechanical phenomena as it does not approximate any correction potential, rather self-consistently solves the basic Schrodinger's equation with Poisson's equation. The only semi-classical point is the effective mass and extension of a single electron wave function to many body theorems. One particular formation of the method adopted in SILVACO simulator is given below,

$$n(r) = \frac{2k_BT}{\pi\hbar^2}\{\sqrt{m_lm_{t1}}\sum_i|\Psi_{li}|^2\ln\left[1 + \exp\frac{E_F - E_{li}}{k_BT}\right] + \sqrt{m_lm_{t2}}\sum_i|\Psi_{ni}|^2\ln\left[1 + \exp\frac{E_F - E_{ni}}{k_BT}\right]$$
$$+ \sqrt{m_{t1}m_{t2}}\sum_i|\Psi_{t2i}|^2\ln\left[1 + \exp\frac{E_F - E_{t2i}}{k_BT}\right]\}$$

$$\nabla\cdot(\varepsilon\nabla U) = q^2[N_D - N_A - n(x)] \quad \text{(2.4b)} \qquad n(r) = \sum_{\infty}|\Psi_\alpha(r)|^2\cdot f_0(\varepsilon_\alpha - E_F)$$

Self-consistent model is vastly used to analyze the behavior of nanoscale devices. It is long been adopted for n-type inversion layer in silicon MOS structure for energy level, population and

charge distribution analysis. The same self-consistent approach has been assumed to describe a cylindrical quantum wire for considering electronic confinement.

3.5. Non equilibrium Greens Function (NEGF) formalism:

This review deals with the non-equilibrium Green's function (NEGF) method applied to the problems of energy transport due to atomic vibrations (phonons), primarily for small junction systems. For quantum mechanical modeling of nanodevices, two formalisms are often used to avoid the huge computational burden of direct solution of the Schrodinger-Poisson approach. One is the Wigner equation commonly solved by finite difference method. A recent study of this equation with Monte Carlo method has shown to resolve both quantum interference and dissipation effect due to scattering. This method has been compared with NEGF formalism based simulator, and found to be equally effective for solving resonant tunneling diodes. This indicates that NEGF is an alternative choice to solving S-P method in quantum devices.

Developing the model

4.1.   Numerical analysis:

Numerical analysis is the area of mathematics and computer science that creates, analyzes, and implements algorithms for solving numerically the problems of continuous mathematics. Such problems originate generally from real-world applications of algebra, geometry, and calculus, and they involve variables which vary continuously. These problems occur throughout the natural sciences, social sciences, medicine, engineering, and business.

Many problems in continuous mathematics do not possess a closed-form solution. In these situations, one has two options left: either one tries to find an approximate solution using seeks a numerical solution. Some problems can be solved exactly by direct methods. However, no direct methods exist for most problems. In such cases it is sometimes possible to use an iterative method. Such a method starts form a guess and finds successive approximations that hopefully coverage to the solution.

4.1.1.   Numerical linear and nonlinear algebra:

This refers to problems involving the solution of systems of linear and nonlinear equations, possibly with a very large number of variables. Many problems in applied mathematics involve solving systems of linear equations, with the linear system occurring naturally in some cases and as a part of the solution process in other cases. Linear systems are usually written using matrix-vector notation, $A\mathbf{x} = \mathbf{b}$, with A the matrix of coefficients for the system, $\mathbf{x}$ the column vector of the unknown variables $x_1, \ldots, x_n,$ and $\mathbf{b}$ a given column vector.

Linear systems are categorized according to many properties (e.g. A may be *symmetric* about its main diagonal), and specialized methods have been developed for problems with these special properties;[2]

Nonlinear problems are often treated numerically by reducing them to a sequence of linear problems. As a simple but important example, consider the problem of solving a nonlinear equation $f(x) = 0$. Approximate the graph of $y = f(x)$ by the tangent line at a point $x(0)$ near the desired root, and use the root of the tangent line to approximate the root of the original nonlinear function $f(x)$.

4.1.2. Solving differential and integral equations:

Most mathematical models used in the natural sciences and engineering are based on ordinary differential equations, partial differential equations, and integral equations. The numerical methods for these equations are primarily of two types. The first type approximates the unknown function in the equation by a simpler function, often a polynomial or piecewise polynomial function, choosing it to satisfy the original equation approximately. Among the best known of such methods is the finite element method (**FEM**) for solving partial differential equations; see [1].

4.2. Finite Element Method (FEM) formation:

The most important factor in numerical solution to Schrodinger's equation is the formation of Hamiltonian matrix. Once done that, the rest part becomes rather trivial to solve. It happens that a quantum system about always constitutes of a number of different energy eigenstates, which in the end gives rise to its own set of system equations. This results effectively in a system of equations. The Hamiltonian in quantum mechanics becomes a matrix for the whole state space and finding the diagonal representation of Hamiltonian remains the major problem. Here gives an example to explain the situation.

When we dealing with a 1D infinite quantum well where an electron is trapped inside, the electron energy will be quantum well will be quantized and it will have a finite probability distribution of occupancy in different eigenstates. But to describe the whole system, all the

29

eigenstates has to be considered. Each eiganstate gives rise to its own wave function which is a solution of the Schrodinger's equation.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \quad (1)$$

Where

$$\hbar = \frac{h}{2\pi},$$

h = Planck's constant,

m = mass of the particle,

ψ = wavefunction

$V(x)$ is a function describing the potential energy at each point x, and

E is the energy, a real number, sometimes called eigenenergy.

For the case of the particle in a 1-dimensional box of length L, the potential is zero inside the box, but rises abruptly to a value V_o at $x = -L/2$ and $x = L/2$. The wavefunction is considered to be made up of different wave functions at different ranges of x, depending on whether x is inside or outside of the box. Therefore the wavefunction is defined such that:

$$\psi = \begin{cases} \psi_1, & \text{if } x < -L/2 \text{ (the region outside the box)} \\ \psi_2, & \text{if } -L/2 < x < L/2 \text{ (the region inside the box)} \\ \psi_3 & \text{if } x > L/2 \text{ (the region outside the box)} \end{cases}$$

Thus the Hamiltonian that describes the Whole system is formed.

$$\begin{bmatrix} \left\{-\dfrac{\hbar^2}{2m_i}\dfrac{\partial^2}{\partial x^2}+U(x)\right\} & 0 & \cdots & 0 \\ 0 & \left\{-\dfrac{\hbar^2}{2m_i}\dfrac{\partial^2}{\partial x^2}+U(x)\right\} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \left\{-\dfrac{\hbar^2}{2m_i}\dfrac{\partial^2}{\partial x^2}+U(x)\right\} \end{bmatrix} \begin{bmatrix} \Psi_1(x) \\ \Psi_2(x) \\ \cdots \\ \Psi_n(x) \end{bmatrix} = \begin{bmatrix} E_1 & 0 & \cdots & 0 \\ 0 & E_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & E_n \end{bmatrix} \begin{bmatrix} \Psi_1(x) \\ \Psi_2(x) \\ \cdots \\ \Psi_n(x) \end{bmatrix}$$

The situation is not resolved. Still a way to discrete the 2nd order differential operator into finite space is needed. A number of ways remain, but the most widely accepted method is Finite Element Method.

As it is considered to be a 1D case only, x is the space dimension. In this case, the function can be expressed as a vector given by:

$$f(x) \Rightarrow \{f(x_1), f(x_2), f(x_3)\ldots\ldots\ldots f(x_{n-1}), f(x_n)\}$$

Then the FEM method finds the 2nd derivative as

$$\frac{\partial^2}{\partial x^2}f(x)\bigg|_{x=x_n} = -f(x_n-1)+2f(x_n)-f(x_n+1)$$

For a 2D case, first a 2D *(n+1)* by *(n+1)* grid is created, where *h=1/(n+1)*is the grid spacing. So the function *U* becomes discrete and the elements *U(I,j)* becomes approximate solutions at *x=i*h* and *y=j*h*

.

The formulation of the 2nd derivative of the point in the middle and the formula is:

$$\nabla^2 U(x)\big|_{x=x_n} = 4U(x_n,y_n)-U(x_n-1,y_n)-U(x_n+1,y_n)-U(x_n,y_n-1)-U(x_n,y_n+1)$$

The above linear equation relating *U(I,j)* and the value at its must hold for *1≤i,j≤n*, giving *N= n^2* equation in *N* unknowns. When *(I,j)* is adjacent to a boundary *(i=1 or i= n or j=n),* one or more of the *U(i±1,j±1)* values is on the boundary and therefore has a value.

4.3. Single Band Effective Mass:

The single-band effective mass Schrödinger equation to calculate the envelope functions is described and its grounds are shown. These envelope functions are used to multiply periodic part of the Bloch functions to obtain approximate eigenfunctions of the Hamiltonian of a nanostructure semiconductor. The Bloch functions, which are the product of a periodic function and a plane wave, constitute the exact solution of a homogeneous semiconductor; they are taken as a basis to represent the nanostructure Hamiltonian. The conditions that make possible the use of this single band effective mass Schrödinger equation are explained. The method is applied to the calculation of the energy spectrum of quantum dots for wave functions belonging to the conduction band.

We shall see that the effective mass equation is only of application when we are dealing with electrons in a single semiconductor band, namely the conduction band. Therefore, the bipolar behavior, in which both electrons and holes enter into or in other words, when electrons in the CB and in the VB.

In the envelope-function method of the wavefunction is written as

$\psi(z) = \Sigma_n Fn(z)U_n(z)$

Where $Un(z)$ are a complete set of functions with the periodicity of the Bravais lattice,and *Fn(z)* is envelope functions with a plane-wave expansion restricted to the firstBrillouin zone. The functions $Un(z)$ are the same throughout the entire structure, hence they cannot be eigenstates of all the local Hamiltonians, and in fact, do not need to. Thewave functions are the solutions of the stationary Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\psi(z) + V(z)\psi(z) = E\psi(z),$$

When *m* the electron mass and *V(z)* the atomic potential of the semiconductor structure. In the k-space, the Schrodinger equation become,

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$$\frac{\hbar^2 k^2}{2m}\tilde{F}_n(k) + \frac{\hbar}{m}\sum_{n'} k \, p_{nn'} \cdot \tilde{F}_{n'}(k) + \sum_{n'}\sum_{k'}\tilde{H}_{nn'}(k,k')\tilde{F}_{n'}(k') = E\,\tilde{F}_n(k),$$

In this case, the Ben Daniel-Duke Hamiltonian is used and the resulting equation is

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m_c(z)}\frac{d}{dz}F_c(z)\right] + V_c(z)F_c(z) = E\,F_c(z),$$

Where $F_c(z)$ is the envelope function for the conduction band, $V_c(z)$ is the potential defining the structure and $m_c(z)$ is the effective mass at z, which in this case is constant within each layer of the basis.

4.4.   Effective mass for Hamiltonian for Hole:

The full-band approach, resulting in multi-band Hamiltonian for holes in the valance band work well for a bulk device. But as it is very much involved with different dimensions, the consequence of using this approach for a nano-device is still somewhat unclear and matter of current research. So far a coarser approximation, one uses the already given effective mass of holes in silicon and constructs an effective mass Hamiltonian for holes to get:

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = -\frac{\hbar^2}{2m^*_{l,h}}\Psi(r,t) + U_v(r,t)\Psi(r,t)$$

Where U_v is the valance band energy and depending upon the particular band, m^* can be for light and heavy hole. The spin interaction band split is ignored for the present purpose.

4.5.   Decoupled set of 1D equation:

In direct discretization, the 2D Schrodinger's equation is considered and using FEM the 2D Hamiltonian matrix is directly created. For example in the case of electron gas, becomes:

$$-\frac{\hbar^2}{2m^*_x}\frac{\partial^2\Phi(x,z)}{\partial x^2} - \frac{\hbar^2}{2m^*_z}\frac{\partial^2\Phi(x,z)}{\partial z^2} + E_c(x,z)\Phi(x,z) = E_l\Phi(x,z)$$

This time instead of trying to directly expand the differential operator according to 2D FEM, the method involves decoupling of dimension variance in an attempt to separate the dimensional dependence.

First a dimension is chosen to start with x. Then starting from one end, say *i=1* mesh points are gradually considered from *U(1,1)* to *U(1,7)* and this 1D system is solved as an eigenvalue problem. This is repeated for every value of *i* till the other end. Then the position dependent eigenvalue *(E₁,E₂...........ect.)* is used as the system potential for 1D systems starting from *j=1* and is solved for points *U(1,1)* to *U(1,7)* and go up to *j=7*. This gives the total 2D solution.
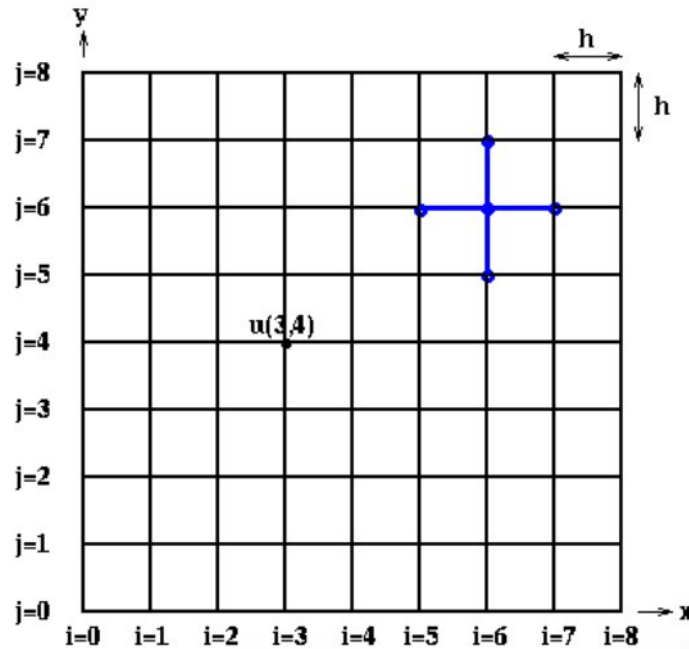
Figure 4.5: Using the discrete 2D mesh for the decoupled 1D system of equations.

As before the starting point is the 2D Schrodinger's equation (the two dimensions being x and z)

$$-\frac{\hbar^2}{2m_x^*}\frac{\partial^2\Phi(x,z)}{\partial x^2}-\frac{\hbar^2}{2m_z^*}\frac{\partial^2\Phi(x,z)}{\partial z^2}+E_c(x,z)\Phi(x,z)=E_i\Phi(x,z)$$

Then the differential equation is expanded in orthonormal basis function such as:

$$\psi(x,y)=\sum_m\delta(x-x')\phi_m(x',y)\varphi_m(x')$$

This actually is quite similar to Fourier analysis.

For thin body, this is about always a good assumption in nano regime, quantum confinement in a particular direction introduces subbands, and only a few subbands are usuallyeffectively occupied. Accordingly, wavefunction is expanded in the already mentioned orthonormal basis.

The eigenfunctions and the associated eigenenergies are obtained by solving a one-dimensional wave equation in the z direction within each x' valued slice.

$$-\frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial z^2}\phi_m(x,z)+V(x,z)\phi_m(x,z)=E_m\phi_m(x,z)$$

It should be noted here that the position dependent eigenvalue is not the eigenstate of the system, as eigenstate does not differ with position in the system.

So algorithm could be described stepwise as follows:

1. Discretize the 2D space coordinates according to the system.

2. Choose a particular direction as the basis function coordinate and expand the wavefunction as below:

$$\psi(x,y)=\sum_m \delta(x-x')\phi_m(x',y)\varphi_m(x')$$

3. Solve for each slice of the chosen coordinate as individual 1D system and the problem reduces to 1D eigenvalue problem:

$$-\frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial z^2}\phi_m(x,z)+V(x,z)\phi_m(x,z)=E_m\phi_m(x,z)$$

4. Using the position dependant eigenvalue from the previous as the potential profile for the other dimension, solve the following equation as another eigenvalue problem:

$$-\frac{\hbar^2}{2m_x^*}\frac{\partial^2}{\partial x^2}\varphi_m(x,z)+V(x,z)\varphi_m(x,z)=E_n\varphi_m(x,z)$$

5. Finally find the overall wave function from the orthonormal basis function expansion given is step 2.

4.6. Green's function:

A significant advancement with the decoupled approach could be attained if the solution method is instead of direct, is the Green's function method. But its advantages are only apparent in complex systems where non ballistic transport is considered with incoherent scattering effects and for a more rigorous contact analysis. It also comes into help if we are trying to simulate a 3D system. But for simpler situation like a 2D infinite potential well, it becomes unnecessarily overburdened.

4.7. Self energy matrix:

For the device the carriers are confined in the lateral direction so that the boundary condition assumes that the carrier concentrations, i.e their wave functions become zero in the silicon-oxide interface. But the longitudinal direction, there are two contacts which in fact inject electrons and holes to the system and have to maintain equilibrium condition for any supplied current. So to incorporate these contacts into the actual device, some modeling method has to be adopted. A very suitable candidate in this case is the self energy matrix modeling the semi-infinite leads.[6]
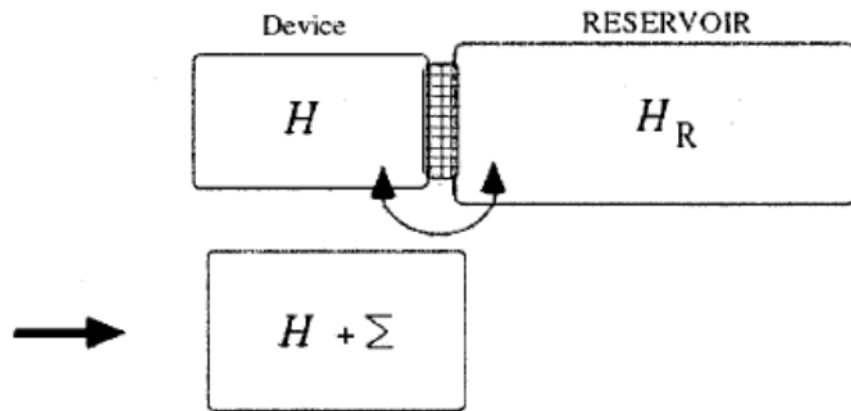
Figure 4.7: Coupling between the contacts (seen as reservoirs of carriers) and the actual device.

The concept of self-energy is used in many-body physics to describe electron-electron and electron-phonon interactions. In the present context, however, it can be used to describe the effect of a semi-infinite contact. In general, a device connected to a large reservoir and has an overall Hamiltonian matrix of

$$\begin{bmatrix} H & \tau \\ \tau^+ & H_R \end{bmatrix}$$

Where the dimension of Hamiltonian for the contact H_R is huge compared to that of the device H.

The overall Green's function has the form

$$\begin{bmatrix} G & G_{DR} \\ G_{RD} & G_R \end{bmatrix} = \begin{bmatrix} (E+i0^+)I - H & -\tau \\ -\tau^+ & (E+i0^+)I - H_R \end{bmatrix}^{-1}$$

36

Here G is related to the device, while G_R is related to the reservoir. The other two are interactions among the two. Because the concern is only about the details inside the device and not inside the reservoir for analysis purposes, only G is of interest (and not in G_R or G_{DR} or G_{RD}). It then becomes is straightforward to show that

$$G = \left[\left(E + i0^+\right)I - H - \Sigma\right]^{-1} \approx \left[EI - H - \Sigma\right]^{-1}$$

Where

$$\Sigma = \tau g_R \tau^+ \text{ and } g_R = \left[\left(E + i0^+\right)I - H_R\right]^{-1}$$

This shows that the effect of the coupling to the reservoir can be accounted for by adding a self-energy matrix Σ to the Hamiltonian H. This is a very general concept that allows eliminating the huge reservoir and working solely within the device whose dimensions are much smaller.

Arbitrary reservoir coupling can be calculated from coupling matrices. [6] So to find the self energy matrix Σ, a huge inversion is required:

$$\Sigma(m,n) = \sum_{\mu,\upsilon} \tau(m,\mu) g_R(\mu,\upsilon) \tau^+(\upsilon,n)$$

The indices m, n refer to points within the device while μ, v refer to points inside the reservoir, so that $g_R(\mu,v)$ for points (μ,v) that are on the surface is needed. This surface Green's function con often be calculated analytically assuming a given reservoir model.

4.8. Bordering effect

If a nano-device is so small that the carriers get confined, then there exit quantized energy states. In itself, this energy distribution can be calculated and accounted for in that device. But whenever a device is mentioned, it is always implied that corresponding contacts are there, as without the contact of the device, which remain the connection of the device to the outer world, the device is of no use. But in the confined nano-device, there is an inherent effect of the contacts on that device. It broadens whatever energy levels the device might have had and must be correctly accounted for device modeling. Depending upon the physical nature of the contact, the

coupling becomes strong or weak, which determines how the levels inside the device will be broadened. It so happens that self-energy method correctly addresses this issue.

Simulation: formulating the model

As the theoretical basis of the device model is gradually constructed, it then remains to implement the model in a simulator to evaluate the performance of the model. The considerations include from choosing of the software to detailed implementation method for different parts.

5.1 Choice of software

Whenever the equation of numerically solving some system of equations arises, the choices become obvious. The effective choice was in choosing one of the mathematical software. The practical choice was in MATLAB, FEMLAB, MATHEMATICA and MAPLE. Among these, the first two are adept to handling floating point operator of complex and huge matrices, while the later two only pose good option for symbolic mathematics. FEMLAB do better job in physical situation involving different systems, as only the Schrodinger's equation has to be solved, MATLAB is as good.

One other important consideration, usually in more practical cases, a device problem should be solved self-consistently, that is iteratively and simultaneously solving Schrodinger's equation with Poisson's equation which at the moment is not possible with FEMLAB.

5.2. Device structure

The device in question is essentially a 2D device. The longitudinal direction is considered to be the x-direction, while the lateral dimension is in the z-direction. y-dimension is the transverse direction and the device is so wide in this direction that the carriers in this direction are free to move and characterized by plane wave. So in essence, the device is distributed in the x-z plane. In the longitudinal direction, the device ends in two contacts, the Anode and the Cathode from where electrons and holes are injected into the device. In the lateral dimension silicon device is sandwiched between two layers of oxide, ensuring confinement in both sides. Half of the device is p type and rest half is n type, so the metallurgical junction is at the middle. Doping is considered to be step type so the junction is abrupt, so that the basic physical effects become

clear. As for device is fabricated in silicon, for confinement, the *z*-dimension is 5nm wide, while in the longitudinal direction, it has a length of 100nm. In *y*-direction, the device is several micrometers wide so effectively it becomes large.
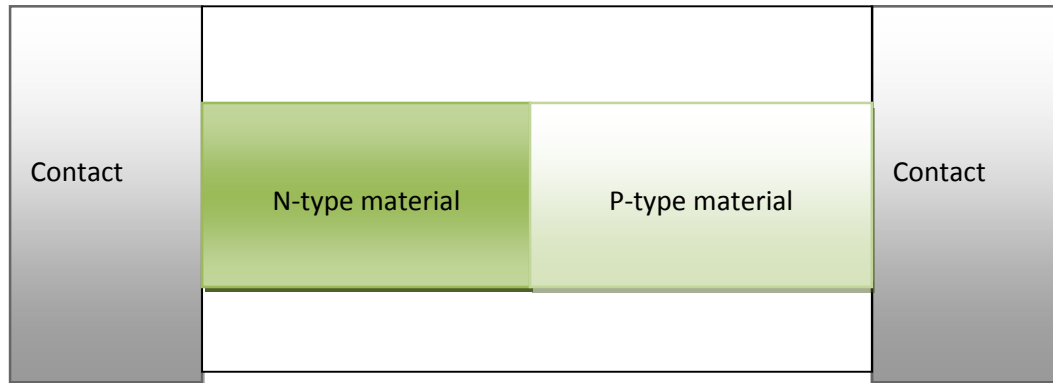

Figure 5.2: Schematic diagram of the device structure in 2D.

5.3. Meshing

Two meshing schemes were considered, the triangular meshing and the rectangular meshing. For triangular meshing, the formulation of 2D Laplacian and the 1D Hamiltonianbecomes involved and the basis physical aspects are curtained, while the rectangular meshing in general has a resolution problem. But the fact that the device is strictly rectangular in shape, made the case for rectangular meshing.

This is for the fact that the actual dispersion relation between energy and discretized momentum of carrier given by

E=2(1-coska)

is well approximated by the continuous dispersion relation

$$E = \frac{n\hbar^2 k^2}{2m^*}$$

5.4. Lateral dimensional Hamiltonian

In MATHLAB, with rectangular meshing for a 1D case in the *z*-direction, an *n by n* Hamiltonian matrix is in order, where n is the number of discrete points in that direction. So if the lateral width is *z* nm and the grid spacing is *a* nm, then *n=z/a*. As n is increased, the size of the matrix also increases and requires more and more computational resource. The coupling constant for the equation is

$$t_z = \frac{\hbar^2}{2m_z^*(\Delta z)^2}$$

Where Δz is the differential distance between mesh points and m_z^* is the z-directed effective mass of concerned carrier, (electron or hole). This is the onsite energy that every particle feels due to lattice, accordingly discredited into FEM formalism.

The device is first sliced into vertical slices of width a so that we have L_x/a vertical slices. It is assumed that all quantities are constant in x-direction within each slice, and a lateral Hamiltonian is constructed for each slice. So for a particular slice, the actual Hamiltonian both for electron and hole becomes:

$$H_z(x_n) = \begin{array}{c c c c c c} & |z_1\rangle & |z_2\rangle & \cdots & |z_{n-1}\rangle & |z_n\rangle \\ |z_1\rangle & 2t_z + U(1,x_n) & -t_z & \cdots & 0 & 0 \\ |z_2\rangle & -t_z & 2t_z + U(2,x_n) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ |z_{n-1}\rangle & 0 & 0 & \cdots & 2t_z + U(n-1,x_n) & -t_z \\ |z_n\rangle & 0 & 0 & \cdots & -t_z & 2t_z + U(n,x_n) \end{array}$$

For example, with *n=5* at the 10th slice, the total Schrodinger's equation in matrix form becomes:

$$\begin{bmatrix} 2t_z+U(1,10) & -t_z & 0 & 0 & 0 \\ -t_z & 2t_z+U(2,10) & -t_z & 0 & 0 \\ 0 & -t_z & 2t_z+U(3,10) & -t_z & 0 \\ 0 & 0 & -t_z & 2t_z+U(4,10) & -t_z \\ 0 & 0 & 0 & -t_z & 2t_z+U(5,10) \end{bmatrix} \cdot \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \end{bmatrix} = \begin{bmatrix} E_1(10) & 0 & 0 & 0 & 0 \\ 0 & E_1(10) & 0 & 0 & 0 \\ 0 & 0 & E_1(10) & 0 & 0 \\ 0 & 0 & 0 & E_1(10) & 0 \\ 0 & 0 & 0 & 0 & E_1(10) \end{bmatrix} \cdot \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \\ \psi_5 \end{bmatrix}$$

For the practical device in consideration, the size is $n=10$.

5.5. Energy Grid

In the longitudinal x-direction, the device is coupled with two contacts, each injecting a particular type of carrier (anode injecting hole and cathode injecting electron). So the Schrodinger's equation is no longer an eigenvalue problem in this dimension, rather the wave functions for given eigenenergy has to be found for a corresponding longitudinal energy. The longitudinal energy is the energy of a carrier in relevant contact that can be injected to the device. Since the device is degenerately doped, the thermal equilibrium Fermi energy lies well within the corresponding band, and particles with any energy between Fermi energy and the band edge can be injected with high probability. So to account for this the longitudinal energy has to be discretized and solution has to be found for all such energy. For longitudinal Hamiltonian, a grid in the energy has to be defined.

For the device in hand, the reference energy is the conduction band energy E_{cn} in the n side. Taking $E_{cn}=0$ then the energy range for electrons remain from 0 to E_{Fn}. Similarly the energy range for the holes is from E_{Fn} to E_{vp}. The energy grid spacing is taken to be $0.5meV$, which is quite typical for such calculations. In equilibrium, $E_{Fn}=E_{Fp}$ while for a bias of V, it is given by $E_{Fn}=E_{Fp}+qV$.
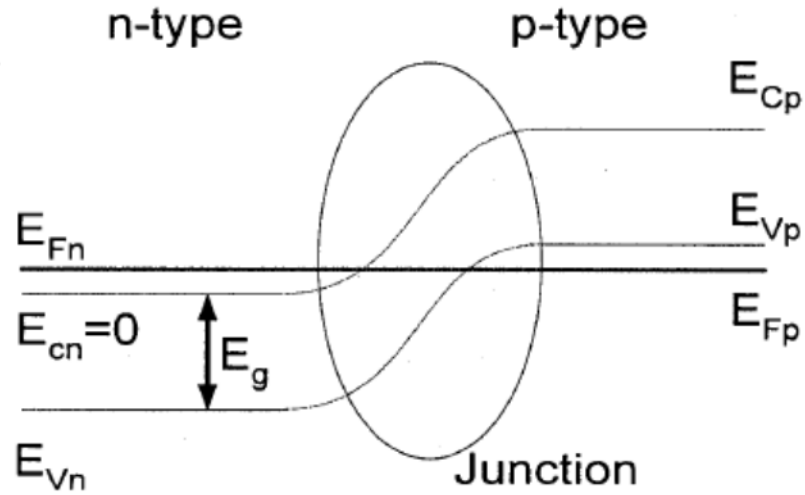
Figure 5.5: The schematic diagram of a p-n junction under equilibrium condition with no bias.

5.6.   Open boundary condition and carrier injection

Semi-infinite contacts are attached to the device as anode and cathode. Because the potential in the contacts is assumed to be uniform, the solutions in the semi-infinite contacts are plane waves. If a unit amplitude wave is injected from the cathode (electron), then some portion reflects from the device and some transmits across and exits the perfectly absorbing anode contact

$$\phi_m(x) = 1e^{ik_x x} + r_m e^{-ik_x x} \ldots\ldots\ldots x < 0$$

and

$$\phi_m(x) = t_m e^{ik_x x} \ldots\ldots\ldots x > L_x$$

Where r_m and t_m are reflection and transmission coefficients for cathode injection into mode m and L_x is the length of the active device.

By solving all equation, the wave function due to the injection of a unit amplitude wave from the cathode is found. This translated to the matrix formation gives the self energy matrices of dimension *n by n* with only one non-zero term

43

$$\Sigma_1(i,j) = -t_x e^{ik_x x} \delta_{1,j} \delta_{1,i}$$

$$\Sigma_2(i,j) = -t_x e^{ik_x x} \delta_{n,j} \delta_{n,i}$$

For carrier injection o source vector term Y_1 is required of *n by I* dimension. It has only one non-zero term is accounting for carrier injection, and also the level broadening.

$$\gamma_1(1) = i\left[\Sigma_1(1,1) - \Sigma_1^*(1,1)\right] = 2t_x \sin k_x a = \hbar \upsilon(k_x)/a$$

So for longitudinal direction the equation that is solved is

$$\left[EI - H - \Sigma_1 - \Sigma_2\right]\phi = -i\gamma_1$$

Similar arguments also account for holes that are injected from anode.

5.7. Steady state carrier density

Electron density for a confined mode *m* and with injected wave vector k_x is obtained from summing all transverse (*y*-directed) mode with wave vector k_y:

$$n_e^m(k_x, x) = \frac{1}{W} \sum_{k_y} |\phi(k_x, x)|^2 f_{FD}\left(E - E_{F,C}\right)$$

Here K_x refers to the X-component of the wave vector of an electron with total energy E in the cathode contact and the probability that the state with total energy E is occupied within the contact is given by the Fermi-Dirac distribution f_{FD}. This is valid because the contacts are always under thermal equilibrium.

The longitudinal summation can also be changed into integral and the final result can be expressed as [].

$$n_e^m(x) = \int_{-\infty}^{\infty} n_e^m(x, E_l)\,dE_l$$

Considering the conduction band (valance band while considering hole calculations) as infinitely wide it can be shown that (including spin delegacy) []

$$n_e^m(x, E_l) = \frac{1}{\hbar a}\sqrt{\frac{2m_y^* k_B T}{\pi}}F_{-\frac{1}{2}}\left(E_{F,c} - E_l\right)\frac{A_e^m(x, E_l)}{2\pi}$$

Here $F_{-1/2}$ is the Fermi integral of order -1/2 and A_e^m is the local density of state:

$$A_e^m(x, E_l) = a\frac{dk_x}{dE_l}\left|\phi_m(x, k_x)\right|^2$$

5.8. Self-consistent analysis

Self consistency is achieved as the successive potential profile difference becomes lower than the preset allowed difference. As the energy grid has been set with a resolution of *0.5meV,* this in fact sets the limit to the maximum achievable accuracy and any error resulting is lesser value is deemed acceptable. This then sets the convergence criteria.

First an initial guess was made for the system potential. The initial guess only plays a part in achieving convergence faster, and for a well formulated problem does not significantly pose a problem. With the guess potential, the quantum transport equations are solved to get the overall carrier density. Then along with the doping profile, this is inputted to the Poisson's equation to get the potential of the system. Then the new potential is compared with the previous potential, and if the difference is larger than the allowed error, the new potential replaces the old one and quantum transport is solved again with the new potential. The process goes on until self-consistent.

5.9. Flowchart

The overall algorithm can be described as follow:

1. Guess a potential profile for the whole system.
2. With this potential profile, calculate the vertical slice confined 1D system equation to get the confined wave function and position dependant eigenenergy.
3. Using the position dependant eigenenergy as the effective local potential, solve the longitudinal system equation with Green's function formation to incorporate contacts and carrier injection.
4. Calculate the carrier density in the device.
5. Using the carrier density and the doping profile, solve Poisson's equation in 2D to find the system potential.
6. Check whether the new calculated potential differs within the given range with the initial potential.
7. If self-consistent is not achieved, repeat above steps.
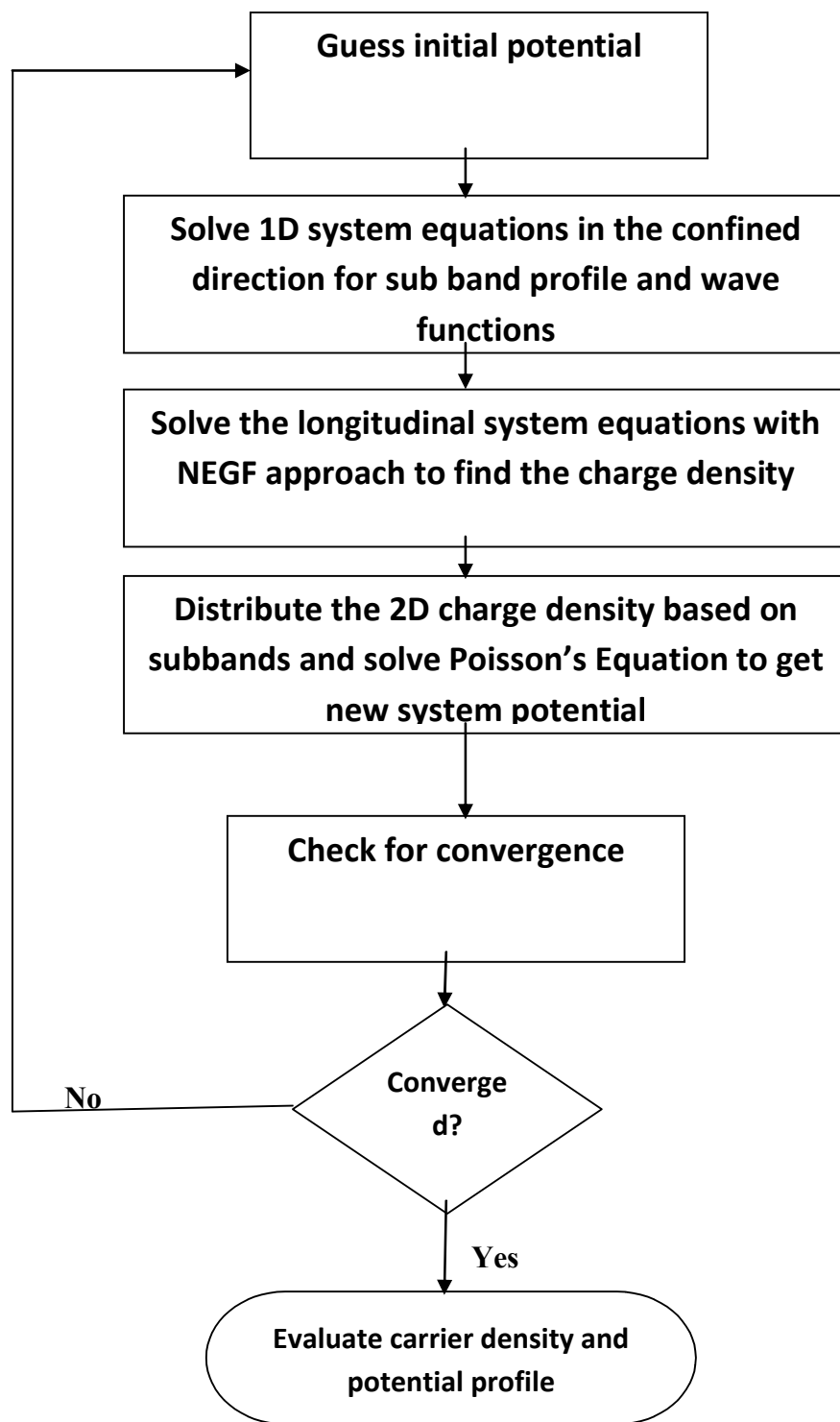8. Once self-consistent is achieved, we calculate relevant properties from carrier density and potential profile.

Figure 5.9: Flow chart of the decoupled system of 1D equation.

CHAPTER-06

Results: Equilibrium potential profile
Built-in potential

A longitudinal section is selected along the device length through the midpoint of the thickness and self-consistent potential is plotted. It can be seen that the difference in potential is plotted. It can be seen that the difference in the n-side and the p-side is the built in potential, V_{bi}, and as for any degenerately doped junction, the magnitude is larger than the band gap energy.
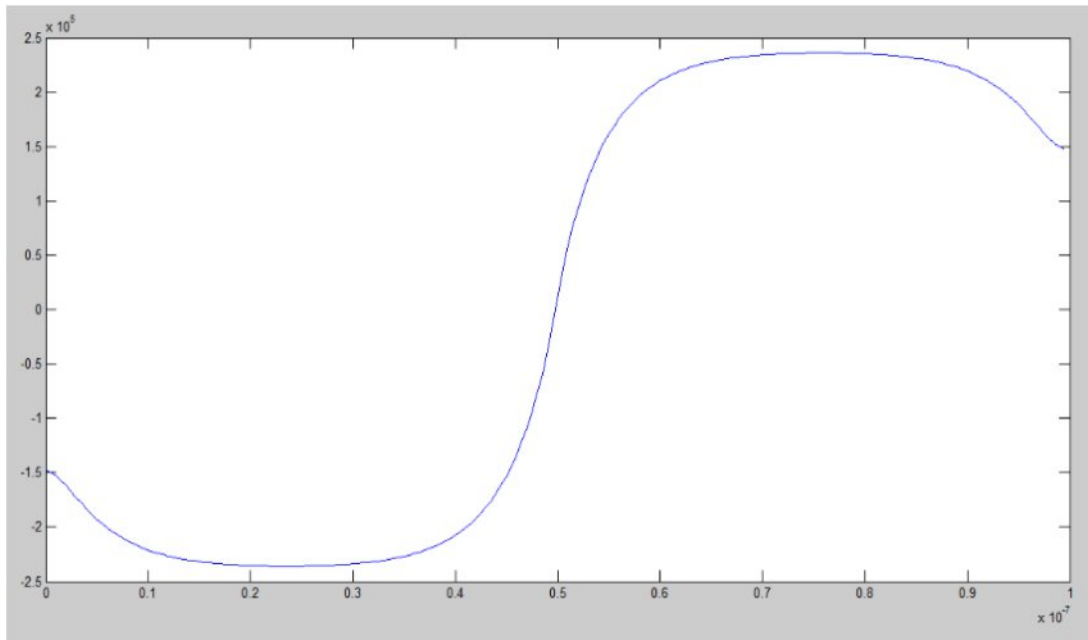

Figure 6.1: Built-in Potential along the device axis (energy vs. device length curve).

In equilibrium, a degenerately doped n-type material will have equilibrium Fermi level within the conduction band. So the Fermi level is situated above the conduction band edge. On the other side, a degenerately doped p-type material will have equilibrium Fermi level within the valance band, hence it will be situated below the valance band edge. Now in equilibrium, it is required that the device the Fermi energy be same, so Fermi energy in the n-type material is exactly equal to the Fermi energy in the p-type material. So the p-type material valance band edge will have

48

higher energy than the n-type conduction band edge. The p-type conduction band being above the p-type valance band by band gap energy, E_g, the difference in conduction band edge between the two sides is given by

$$\Delta\text{◻} = E_{cn} + E_{Fn} + E_{Fp} + E_g$$

So the built in potential is given by

$$V_{bi} = E_{Fn} + E_{Fp} + E_g$$

Depletion region:

Rise in potential which is equal to the built in potential, is in fact the depletion region, where the material is depleted of free carriers. The length of the depletion region is calculated from the point where the potential starts to rise till the point where the potential becomes constant again. It can be seen that the value of the depletion region width is about one order more than predicted by 3D equations
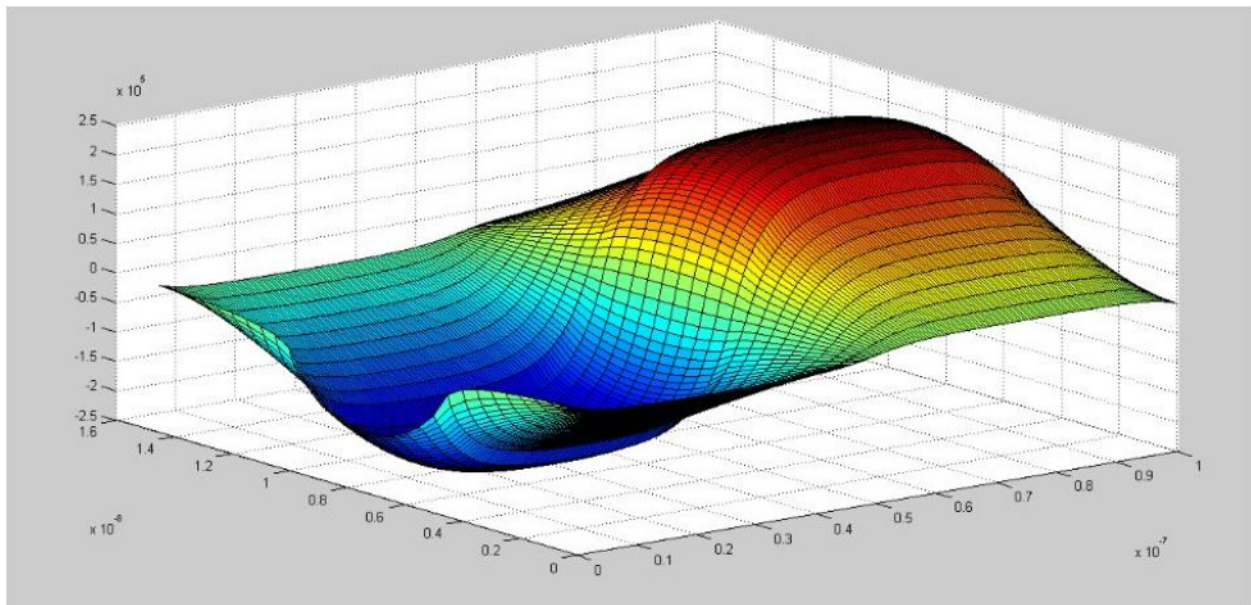

Figure 6.2: Conduction band of the 2D p-n junction in silicon (3D).

CONCLUSION

There has been considerable work on developing quantum transport model for unipolar device structures like MOS, but not on bipolar devices. Most of these works concentrate on electron as carrier and at least, sometimes consider holes as the sole carrier. But in p-n junction, both electrons and holes exit and create junction with associated depleted region, which then creates the basis device.

It could be pointed out that the contribution of this work could be listed as follows:

- The 2D Schrodinger's equation is decoupled for a bipolar system into a set of 1D equation and applied simultaneously to electrons.
- A simulation model of 2D p-n junction in silicon is developed.
- Simulation is carried for both equilibrium and biased condition.

REFERENCES

1. O'Mara, William C. (1990). *Handbook of Semiconductor Silicon Technology*. William Andrew Inc. pp. 349–352. ISBN 0-8155-1237-6.

2. NNDC contributors (2008). Alejandro A. Sonzogni (Database Manager), ed. "Chart of Nuclides". Upton (NY): National Nuclear Data Center, Brookhaven National Laboratory. Retrieved 2008-09-13.

3. "Chapter 6: Diodes." Fundamentals of Electrical Engineering. 2nd ed. New York, New York: Oxford UP, 1996. 352-54. Print.

4. http://www.electronics-tutorials.ws/diode/diode_3.html

5. Jackson, Julia A.; Mehl, James P.; Neuendorf, Klaus K. E., eds. (2005), *Glossary of Geology*, American Geological Institute, Springer, p. 503, ISBN 978092215276

6. http://www.electronics-tutorials.ws/diode/diode_2.html

7. http://www.circuitstoday.com/pn-junction-diode-characteristics

8. http://www.daenotes.com/electronics/basic-electronics/energy-band-insulator-conductor-semiconductor

9. http://www.dummies.com/how-to/content/translate-the-schrodinger-equation-to-three-dimens.html.

10. S. Brenner and L. Scott (1994)"The Mathematical Theory of Finite Element Methods," Spring-Verlag.

11. J. Dongarra, I. Duff, D. Sorensen, and H. van der Vorst (1998) *Numerical Linear Algebra for High-Performance Computers*, SIAM Pub.

12. K. Atkinson (1997) *The Numerical Solution of Integral Equations of the Second Kind*, Cambridge Univ. Press.

13. Datta S (1989) Quantum phenomena. Molecular series on solid state devices, vol 8. Addison Wesley, Reading

14. Kaxiras E (2003) Atomic and electronic structure of solids. Cambridge University Press,New York.

15. S. Datta, "nanoscale device modeling: the green's function method", Supperlattices and Microstuctures, Vol. 28, No. 4, 2000.

16. Roger A. Faulkner, "Toward a Theory of Isoelectronic Impurities In Semiconductors"; Physics Review, Vol.175,pp991-1009,1968.

17. C. Pickering,M.I.j. Beale, D.J. Robbins, P.J. Pearson, R. Greef, "Optical studies of the structure of porous silicon films formed in p-type degenerate and non-degenerate silicon"; Journal of Physics C; Solid State, Vol.17, No.35, pp 6535-6552, 20 December 1984.

18. V. Lehmann, U. Gosele, "Porous silicon formation: A quantum wire effect"; Applied Physics Letters, Vol.58, Issue8, pp. 856-858, 25 February, 1991.

19. S. Datta, "Quantum Transport: Atom to Transistor"; Cambridge University Press.

20. F. Stern, "Self-consistent results for n-type Si inversion layers"; Physical Review B, Vol. 5, No.12, June 15, 1972.

21. http://www.mathworks.com/matlabcentral/fileexchange/38090-2d-poisson-equation/content/Poisson_equation_2D.m.

22. www.matlabworks.com.

23. L. Shifren,D.Feery,"Winger function quantum Monte Carlo"; Physica B, Vol.314,pp. 72-75,2002.

APPENDIX

Sample MATLAB code:

```matlab
clc; clear all;
Length=1e-7;  %Device length in x direction
Thickness=5e-9;  % Device thickness in z direction
Width=5e-6;     %Device width in y direction
Oxide=5e-9;  % oxide thickness in z direction

a=5e-10;   %slice width
b=5e-10;    %Mesh point distance in each verticle slice
c=5e-10;     %mesh point distance in oxide
mode= 5;     % number of subbands to be consider
Volt= 1.4; % applied voltage


%  constant....
K=8.61735E-5;     %Boltzman constant
q=1.6e-19;          %electronic charge
hbar=1.0544e-34;  %Reduced Plank's conostant
mex=0.916;         %Effective electron mass in X direction
mey=0.916;         %Effective electron mass in Y direction
mez=0.916;         %Effective electron mass in Z direction
mpx=0.916;          %Effective hole mass in X direction

mpy=0.916;         %Effective hole mass in Y direction
mpz=0.916;         %Effective hole mass in Z direction

melec=9.1e-31;     % Electron rest mass in kg
T=300;
epsilon0=8.8542e-12; %permittivity of free space
epsilonr=11.8;        %relative permittivity of silicon
epsilonox=12.8;      %relative permittivity of oxide


Nx=round(Length/a);  % number of vertical slices
Nz=round(Thickness/b);  %number of nodes in device slice
Nox=round(Oxide/c);   %number of oxide
Nthick=Nz+2*Nox;      %number of nodes in each vertical slice
kt=K*T;
Ae=2*mez*melec/(hbar)^2;  %coefficient of electron Schrodinger eq.
Ap=2*mpz*melec/(hbar)^2;   %coefficient of hole Schrodinger eq.
```

```matlab
tez=(hbar^2)/(2*mez*melec*b^2*q);  %electron coupling conostant
tex=(hbar^2)/(2*mex*melec*a^2*q);  %electron coupling conostant
tpz=(hbar^2)/(2*mpz*melec*b^2*q);  %hole coupling conostant
tpx=(hbar^2)/(2*mpx*melec*a^2*q);  %hole coupling conostant

Efn=0.4;                %Fermi energy of anode(referance value)
Ecn=0.001;               %conduction band of cathode side
Efp=Efn-Volt;            %Fermi energy of cathod(referance value)
Ecp=0.001;               %conduction band edge of n side
Em=zeros(Nx,mode);         %energy in each vertical side
U=zeros(Nthick,Nx);       %protential profile
Eleamax=0.125;           % maximum injection energy for electron from anode
Eleamin=Ecn;            % minimum injection energy for electron from anode
Elecmax=0.125;           %maximum injection energy for electron from cathode
Elecmin=Ecp;            %minimum injection energy for electron from cathode
Eldiff=5e-4;           %energy grid spacing
Elp_max=0.8*tpx;
Elp_min=0.001;
Elp_diff= 5e-4;
sigma1=zeros(Nx);
sigma2=zeros(Nx);
gama1=zeros(Nx,1);
nelec=zeros(Nx,mode);   %electron concentration in the device
nhole=zeros(Nx,mode);
NE_anode=round((Eleamax-Eleamin)/Eldiff);

NE_cathode= round((Elecmax-Elecmin)/Eldiff);

NP=round((Elp_max-Elp_min)/Elp_diff);



%Eigenfunction in each vertical slice

phiz=zeros(Nx,Nz,mode);
phixa=zeros(round((Eleamax-Eleamin)/Eldiff),Nx,mode);
phixc=zeros(round((Elecmax-Elecmin)/Eldiff),Nx,mode);
nanodemode=zeros(Nx,mode);
nanodem=zeros(Nx,Nz,mode);
nanode=zeros(Nz,Nx)';
ncathodemode=zeros(Nx,mode);
ncathodem=zeros(Nx,Nz,mode);
ncathode=zeros(Nz,Nx)';
eprob=zeros(Nz,Nx)';
nelec=zeros(Nx,Nz);        %2 dimensional density
nhole2D=zeros(Nx,Nz,mode);
```

```matlab
nhole3D=zeros(Nz,Nx)';
phole3D=zeros(Nz,Nx)';
u =U;
epsilon=epsilon0*epsilonr;
epsilonx=epsilon0*epsilonox;


%  2dpoisson' Eqation

d=zeros(Nthick+2,Nx+2);
ind=1;
forjj=2:Nthick+1;
for ii=2:Nx+1;
d(jj,ii)=ind;
ind=ind+1;
end
end
d=-delsq(d);

% Nx, Nox, Nz
for ii=(Nx*Nox)+1:Nx:Nx*(Nox+Nz);
d(ii,ii)=-3;
d(ii,ii-1)=0;
d(ii+Nx-1,ii+Nx-1)=-3;
ifii+Nx<4001
d(ii+Nx-1,ii+Nx)=0;
end
end



dinv=inv(d);

%Energy grid for longitudinal Energy


Elea=linspace(Eleamin,Eleamax,round((Eleamax-Eleamin)/Eldiff));
Elec=linspace(Elecmin,Elecmax,round((Elecmax-Eleamin)/Eldiff));

%Doping profile calculation

Ndevice=-(1e21)*ones(Nz,Nx);
for ii=1:Nx/2;
Ndevice(:,ii)=1e21;
end
```

```matlab
% self consistent solution

for mm=1.4:1.4;
   Volt=mm;
itteration=1;
error=inf;
check=1;
while error>Eldiff
Uold=U;
%Device Potential

Udevice(:,:)=U(Nox+1:Nox+Nz,:);
Uave=mean(Udevice);      %for carrier injection
%Hamiltonian matrix for each vertical slice

for ii=1:Nx;
   hz=2*tez*diag(ones(1,Nz))-(tez*diag(ones(1,Nz-1),1))-(tez*diag(ones(1,Nz-1),-
1))+diag(Udevice(:,ii));
   [V,D]=eig(hz);
forjj=1:mode; %For each mode in a particle slice...

     phiz(ii,:,jj)=V(:,jj); %eigenenergy of each mode at different slices
Em(ii,jj)=D(jj,jj);
eprobm=abs(phiz(ii,:,jj)).^2;
end
end

% Hamiltonnian matrix in longitudinal direction
for ii=1:round((Eleamax-Eleamin)/Eldiff);  %for each energy
coska=1-((Elea(ii)-Uave(1))/(2*tex));
ka=acos(coska);
sigma1(1,1)=-tex*exp(i*ka);
coska=1-((Elea(ii)-Uave(Nx))/(2*tex));
ka=acos(coska);
sigma2(Nx,Nx)=-tex*exp(i*ka);
   gama1=diag(i*(sigma1-sigma1'));
    gama2=diag(i*(sigma2-sigma2'));
forjj=1:mode;
     hx=(2*tex*diag(ones(1,Nx))+diag(Em(:,jj)))-(tex*diag(ones(1,Nx-1),1))-
(tex*diag(ones(1,Nx-1),-1));
     G=Elea(ii)*eye(Nx)-hx-sigma1-sigma2;
phixa(ii,:,jj)=-i*G\gama1;
     G2=Elec(ii)*eye(Nx)-hx-sigma1-sigma2;
phixc(ii,:,jj)=-i*G2\gama2;
```

```matlab
        n(:,jj)=((sqrt(2*mey*melec*kt/pi))*(abs(phixa(ii,:,jj)).^2)*(fermi((Efn-Elea(ii)),-
0.5)))/(hbar*2*pi*gama1(1,1));
         p(:,jj)=((sqrt(2*mpz*melec*kt/pi))*(abs(phixc(ii,:,jj)).^2)*(fermi((Elec(ii)-Efp),-
0.5)))/(hbar*2*pi*gama2(200,1));

end
nanodemode=n+nanodemode;
ncathodemode=p+ncathodemode;
end

%Calculating 2D electron density


for ii=1:Nx;
forjj=1:mode;
nanodem(ii,:,jj)=nanodemode(ii,jj)*((abs(phiz(ii,:,jj))).^2);
         ncathodem(ii,:,jj)=ncathodemode(ii,jj)*((abs(phiz(ii,:,jj))).^2);

end
end
for ii=1:mode;
nanode=nanodem(:,:,ii)+nanode;
ncathode=ncathodem(:,:,ii)+ncathode;
end


%Poisson's equation

rho=[zeros(Nox,Nx);(nanode'-ncathode'-Ndevice);zeros(Nox,Nx)];
rhovect=reshape(rho',[],1);
     u=dinv*rhovect;
beta=-q*a^2/epsilon;

     u=beta*u;

U=reshape(u,[],Nthick)'./[epsilonx*ones(Nox,Nx);epsilon*ones(Nz,Nx);epsilonx*ones(Nox,Nx)
];
error=max(abs(U-Uold));
end
end

% x=U(:,Nx);
% y=U(:,Nox);
% [xx,yy]=meshgrid(x,y);
x=(0:1:Nx-1)*a;
```

```matlab
y=(0:1:Nthick-1)*c;

surf(x,y,U);

% figure;
% surf(xx,yy);
% xlabel('U_x axis')
% ylabel('U_y axis')
% axis tight
% shading interp
% colorbar
```

END