MONTE CARLO SIMULATIONS OF IONIZED IMPURITIES PROFILE IN A SEMICONDUCTOR IN EXTERNAL PARABOLIC POTENTIAL

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Acronyms

V_o = external potential amplitude

nstp = number of time steps

T = temperature

NP = number of impurity per site at the initial

initial p.t = initial point or at 1 step (ground)

K = Kelvin (the SI unit of temperature)

V = volt (the SI unit of potential)

U = potential energy in eV

Abstract

In this thesis we have investigated impurities profiles in a semiconductor layers, using Monte Carlo simulation technique in an external parabolic potential. By ignoring impurity - impurity Coulomb's interaction, first we considered impurities diffusion in the presence of external parabolic potential that has minimum at the center of the semiconductor at a different temperatures. The model was modified and included the impurity impurity Coulomb's interaction. Using Arrhenius type equation, we have performed Monte Carlo simulation to predict impurities profile for different amplitudes of external parabolic potential, temperatures and impurities density per sites. When we approximated the non - linear potential as one dimensional parabola which has a minimum at the mid point of the semiconductor layer, the impurity is accumulated in the central region. Our results show that the external potential has influenced the diffusion towards the center even though an internal potential has opposite effect. Moreover the impurity distribution has a Gaussian profiles that becomes sharper when the amplitude of external parabolic potential is increased. Our simulation results were compared with the pervious related works. The variation of the gaussian width within a temperature and dopant density per site were also observed that as the temperature increases the plots becomes broaden. Similarly, as the dopant density per site at the initial increases the impurities per site around the center of the graph becomes higher and broaden.

Chapter 1
Introduction

Early experiments with semiconductors were viewed as a family of solids with irreproducible properties. But through a scientific efforts overcame this idiosyncrasy and turned by the art of impurity doping into versatile applications of an important and reproducible technology [1]. Impurity doping in a semiconductor material is emerging now a days as a useful and reproducible technology that has been exploited to control opto electronic properties of a wide range of semiconductor devices [2]. Proper understanding of the fundamental physics of impurity diffusion in a semiconductor has great significance for technology. The technology uses an impurities profiles which has applications in electronic devices [3, 4]. Electronic dev-ices are tools (materials) that control a flow of electrons and they can be used as main (basic) building blocks of all electronic circuits, as a result, devices made from semiconductors are important for the construction of modern electronic equipment. One of the significant features of the semiconductor is the possibility to adjust their conductivities by introducing impurities (dopants) into their crystal lattice [4, 5].

The desired physical and electrical proprties of electronic materials are generally obtained by processing at elevated temperatures, and then understanding of all the changes that occur during these process is based on a knowledge of impurities diffusion in semiconductors [6]. Impurities are generally introduced at high tempratures by the techinques of ion implantation [4, 7], and diffusion [7, 8]. Impurities are distributed in a semiconductor when the semiconductor crystal is heated to a high temperature, many of the crystal atoms can randomly move in and out of their single crystal lattice sites and then Vacancies may be created by this random motion that impurity atoms can move through the lattice by hopping from one vacancy to another. When the temperature decreases, the impurity atoms become permanently frozen into the substitutional lattice sites. Diffusion of various impurities into selected regions of a semiconductor allows us to fabricate complex

electronic circuits in a single semiconductor crystal. Impurities are also introduced by ion implantation when a beam of impurity ions is accelerated to high kinetic energies and then directed (injected) to the surface of the semiconductor. The high energy impurity ions enter to the crystal and come to rest at some average depth from the surface. One advantage of ion implantation is that controlled numbers of impurity atoms that can be introduced into a specific regions of the crystal and processed at lower temprature compared to diffusion. Similarly, the disadvantage of this technique is that the incident impurity atoms collide with the crystal atoms which is causing lattice displacement and damage [9]. Therefore methods of forced diffusion introduction of impurity is more pereferable than ion implantation. Although the impurities are most of the time introduced by ion implantation, which has structural defects that are difficult to cure so, the physics of thermal diffusion of the impurities along the semiconductor layer has attracted considerable attentions [10, 11]. Both methods forced diffusion and ion implantation assisted doping during growth of diamond thin film technology in reproducible production of p-n junctions, introduce no additional structural defects, except that inherent to the impurity itself [12].

Studies of impurity diffusion in semiconductor layers showed that the conductivity of these semiconductors can be manipulated by varying the carrier concentration of impurities as well as the background of temperature along the semiconductor layers. And the level of conductivities can be controlled by the amount and type of impurities. To increase conductivity of semiconductors the band gap of the material should be decreased (lower). When the amount of impurity added is small the crytal structure of semiconductor is not disturbed then impurity behaves like individual atom and do not form cluster but if we increase quantity of impurity in semiconductor, the amount of carrier concentration will increase equally the conductivity of semiconductor increase. As the background of temperatures steps up the diffusivity of the impurities is increased, similarly the number of charge carriers also increases, and consequently contrary to conductors the conductivity increases. On the other hand when the background temperature of the semiconductor layer is far from frozen temperature the impurities (either accepters or donors) diffuse through the semiconductor layer. Therefore manipulating the diffusivity of these impurities to a desired region along the semiconductor layer is vital and has received considerable attentions [4, 13].

Some of the studies have also revealed (proposed) as the way of controlling impurity diffusion by applying a controllable external harmonic potential energy [10, 13], when the external potential energy is exerted it compels the particles to accumulate around its potential minima. The location of the high density region is linked to the shape of the external field. The external parabolic potential has its minimum at the center of a given organic semiconductor layer. This potential can be formed by splite gates. When the external parabolic potential from the gate is increased, it showed that this potential overcomes the internal potential for a given doping concentration. it confines the particles to accumulate around its center (potential minima). On the other hand when the gate voltage potential is off, there is no external potential and the charge carriers are distributed and free to move over all the layers. Conversely, if the gate voltage is on (and also high enough), the charge carriers are confined to the center and the current does not flow [10, 13, 14]. Hence by controlling the external potential(potential minima) along the layer, one can control the profile of the impurity without increasing the background temperature which in turn has an advantage of preserving the crystal structure as diffusion takes place at lower temperature [5, 12, 14].

A model in which an external one dimensional parabolic potential defined by split gates is used to calculate impurities profile in a semiconductor layer. The impurities profile can be widely altered by changing the temperature, the average doping density, the size and the parabolic external potential amplitudes. At high temperatures the impurities are ionized and are able to move relatively quickly, after a realistic equilibrium time, the profiles are rapidly cooled such that the impurities are frozen in place. The impurities profiles are typically Gaussian shaped, where the distribution broadens with increasing temperatures. They are sharper as theparabolic external potential amplitude increases and the processing temperature is lowered. The processing time, however, is increasng exponentially as the temperature is lowered, and this must be considered in the practical situation. Neglecting the interaction between the dopants at low impurity density, it was showed that the diffusion of impurities can be controlled by varying the external potential and by altering the intensity of temperature of the impurities.

The objective of the present study is to show how impurities diffuse along semiconductors in one dimesional external parabolic potential, numerically using Monte Carlo (MC) simulation methods. An external parbolic potential, density of impurity and temperature are the parametr-es used in this study. We used Arrhenius type equation as a centeral equation in our model to describe the diffusion process of impurities. The Arrhenius equation is modified to include the position dependant potential to drive the hopping probabilities. Impurities without external field has equal chance of hopping in all directions. But the potential biases the hopping towards the lower potential, the minimum potential energy point being the minima of the external parabolic potential. We have written Fortran 90 program code to perform Monte Carlo simulation in order to determine the density profiles. We got results and compared them with the results in literature and proposed an experiment for this verification.

The rest of this thesis is organized as follows. Chapter two will discuss the overview of the semiconductors, type of semiconductors, doping in semiconductors and diffusion theories. Chapter three presents the model and method. In Chapter four, we will present the results and discussion of our Monte Carlo simulations(MC) results. The summary and conclusio-n is presented in Chapter five.

CHAPTER 2

Over view of impurity diffusion in semconductors

2.1 Semiconductors

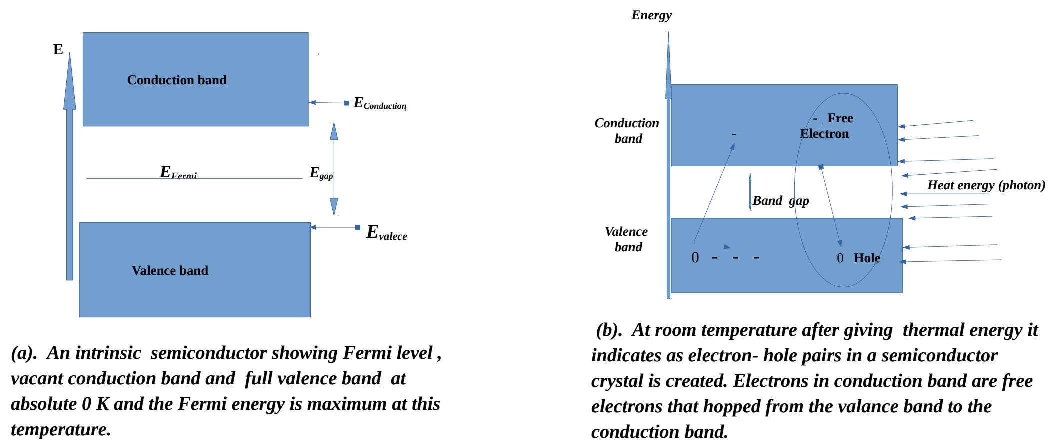
A semiconductor is a material that is between conductors and insulators in its ability to conduct electrical current. Two general classifications of semiconductors are the elemental semiconductor materials found in group IV of the periodic table characterized by atoms with four valence electrons, such as silicon and germanium and the other classification is compound semiconductor materials, most of which are formed from special combinations of group III and group V elements like gallium arsenide, indium phosphide, gallium nitride and silicon carbid. The resistance of semiconductors fall as their temperatures raised which is in opposite to metals (conductors). Which means that conductivity of semiconductors increase either by increasing temperature or inctroducing impurities.

The properties of electric conduction of a semiconductor alters in to useful way by introducing impurities (by doping) in to crystal structure. Semiconductor materials play a major role in high technique equipment used in industry and in daily life. Silicon (Si) is one of the most important semiconductor for the fabrication of micro-electronic devices such as memory and processor chips for computers and solar cells for energy production in photovoltaic devices. Germanium (Ge) is also another inorganic semiconductor that constitutes the base material for gamma radiation detectors. Gallium arsenide (GaAs) and other compounds of group III and group V elements of the periodic table are mainly used in optoelectronic and high frequency devices such as solid state lasers in compact disc players and receivers in cellular phone. Silicon carbid is a semiconductor with a large band gap and has potential for applications in devices that must be operated at high temperatures, high frequencies and under irradiation [6, 9].

The conductivity of silicon is increased by adding a small amount of (1 percent for 10^8 percent) of pentavalent like antimony, phosporus and arsenic or trivalent like boron, gullium, indium atoms. This process is known as doping resulting to extrinsic semiconductors. Conductivity of semicondutors can also be improved by increasing its temperatures, contrary to metals whose conductivity decrease as temperature increases. High conductivities in material comes from its partially filled states and state of delocalzation. Then Metals have many partially filled states with energies near their Fermi level and present electrons in state to conduct electricity. Semiconductors by contrast have few partially filled states Fermi level sit within band gap with few energy states to occupy and blocking the passage of electrons via that state. Band gap (energy gap E_g) is the difference in energy between the lowest point of conduction band, which is vacant called conduction band edge, and the highest point of valence band, that is full called valence band edege, at absolute temperature. As the temperature steps up the electrons thermally excited from the valence band to the conduction band. Both the electrons in the conduction band and the holes left in the valence band have contributed for the electrical conductivity. In the low temperature range the electrical properties of semiconductors are not essentially modified by impurities in the crystal [15].

2.1.1 Instrinsic (undoped) semiconductors

Intrinsic semiconductors also known as undoped semiconductors that have large energy gap compared to doped semiconductor elements. The number of charge carrier is therefore determined by the properties of material itself instead of the amount of impurities. In the case of intrinsic semiconductors the number of excited electrons and number of holes are equal (n = p). At absolute temperature intrinsic semiconductors form very strong covalent bond to each other and there are no free electrons due to that acts as insulator. But an intrinsic crystal semiconductors at room temperatures have sufficient heat (thermal) energy for some valence electron to jump the gap from the valence band into the conduction band, becomes free electrons. Free electrons are also called conduction electrons like that in Fig.2.1(b).



(a). An intrinsic semiconductor showing Fermi level , vacant conduction band and full valence band at absolute 0 K and the Fermi energy is maximum at this temperature.

(b). At room temperature after giving thermal energy it indicates as electron- hole pairs in a semiconductor crystal is created. Electrons in conduction band are free electrons that hopped from the valance band to the conduction band.

Figure 2.1: (a). The conduction band is vacant, valence band is full at initially and (b). It shows as electrons jump from valence band to conduction band [16]

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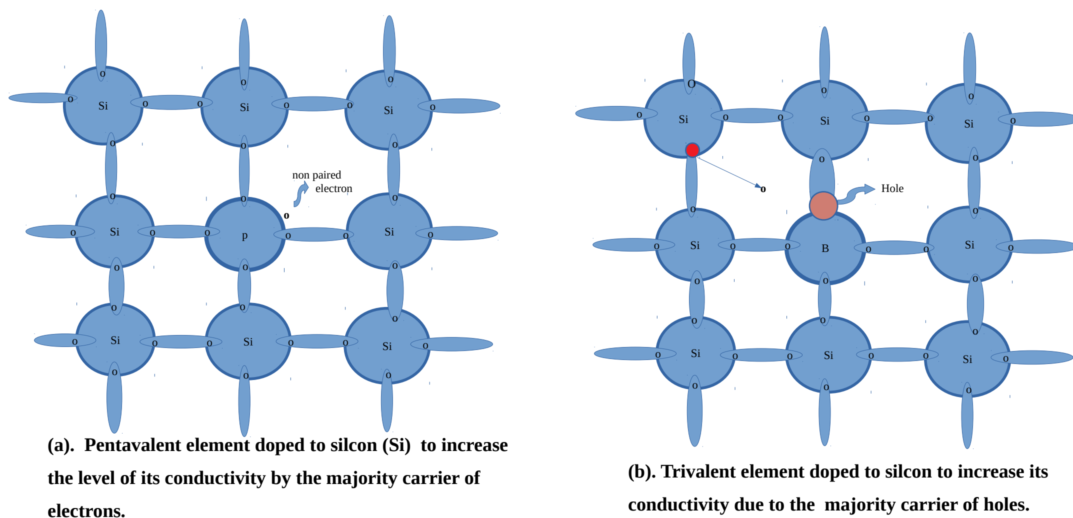
2.1.2 Extrinsic(doped)semiconductors

In semiconductor production doping is the intentional introduction of impurities in to an intrinsic semiconductor for the purpose of modulating its electrical, optical and structural properies. This semiconductor called extrinsic semiconductor. In an extrinsic (doped) semiconductors, dopant atoms increase the majority charge carrier concentration by donating electrons to the conduction band or by producing holes in the valence band, hole is a position where electron is missing that can behave majority carreir concentration by accepting electrons. When the concentration of dopant atoms added is small compared to the density of semiconductor atoms, the small number of impurity atoms are spread far enough apart so that there is no interaction between donor electrons. Then we assume that the impurities introduce discrete and non interacting donor energy states in the n-type semiconductor. In similar process non interacting accepter states can be thought in the p-types of semiconductors. These type of semiconductors are refered to as non degenerate semiconductors. On the other hand, if the impurity concentration

increases the distance between the impurity atoms decrease and will be reached when the donor electrons will begin to interact with each other. When this occurs the single discrete donor energy will split in to a band of energies. As donor concentration further increases the band of donor state widens and may overlap with the bottom of the conduction band. This over lap occurs when the donor concentration becomes comparable with the effective density of states. When the concentration of electron in the conduction band exceeds the density of state the fermi energy locates within the conduction band, this type of semiconductors called a degenerate n-type semiconductor, similarly when the concentration of holes exceeds the density of state, this type is also called a degenerate p-type semiconductor. Impurity doping emerges, due to the mingling of new confinement sources with impurity related potentials. Such confinement coupled with the dopant location can dramatically alter the electronic and optical properties of the system. Without impurities, there would be no diode, no transistor or no semiconductor science and technology [2].



(a). Pentavalent element doped to silcon (Si) to increase the level of its conductivity by the majority carrier of electrons.

(b). Trivalent element doped to silcon to increase its conductivity due to the majority carrier of holes.

Figure 2.2: (a). Doped semiconductors, which is pentavalent phosphur doped to silicon semiconductor and
(b). Doped semiconductor which is trivalent Boron doped to silicon [16]

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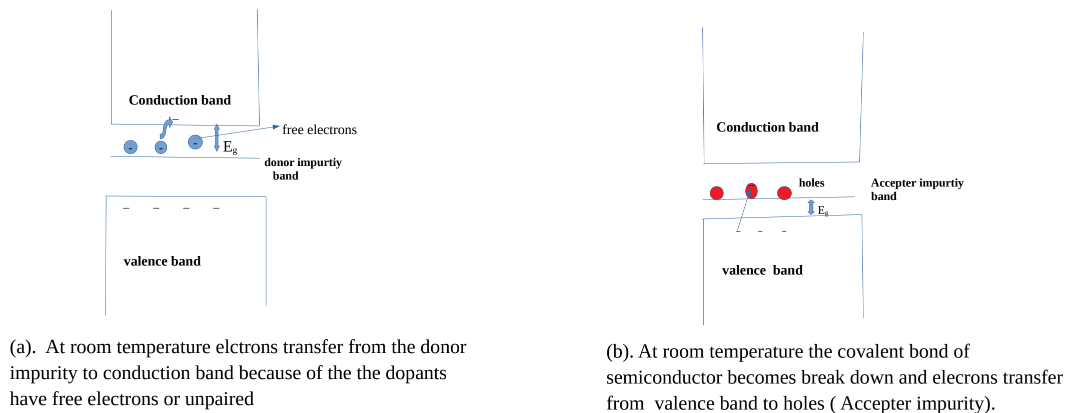
During doping process, dopants get position in crystal lattice of the semiconductor. It is important that the dopant does not distort crystal lattice of semiconductor. From this the dopant atoms of the semiconductor crystal should be comparable to the semiconductor atoms in size. The intrinsic semiconductor (Si) form four covalent bond for both surrounding of each atoms. The addition of pentavalent and trivalent dopants create two different types of extrinsic semiconductors. When a pentavalent dopant phosphur (P) is doped to silicon semiconductor crystal lattice, a pentavalent dopant in crystal lattice of semiconductor forms covalent bond with four neighbouring atoms of semiconductor as we observe in Fig.2.2(a). A pentavalent atom still has one very losly bound valence electron that can be set free using very small amount of energy. Thus each pentavalent dopant atom contributes a free electron to the crystal lattice semiconductor. Therefore number of free electrons that available for conduction by doping atoms depends lastly on the level of doping. If doping level is high number of free electrons contribute for conduction by the dopants increase. This number of free electrons contributes by the donor dopant is not depended on the temperature of semiconductor crystal. On the other hand if temperature of crystal increases number of intrinsic electron hole pairs increase and this further as to the conductivity of the crystal. Hence in semiconductor doped with pentavalent dopants the total number of conduction electrons is due to a free electron contributes by the donor atoms which are pentavalent dopants and lose generates intrinsically. But total number of holes is only due to a hole from the intrinsic source. Due to the increasing in number of free electrons the rate of recombination of holes increase. This gives like to the reduction in number of holes effectively. As compare to the number of free electrons available for conduction the number of free electrons in semiconductor doped in the pentavalent dopant is much larger than the number of intrinsic holes. Negative charge of free electrons act as majority charge carrier in a semiconductor doped with a pentavalent dopants. Thus such extrinsic semiconductor called n-type semiconductor. When dopant atom in n-type semiconductor gives valence electron it becomes positively charge. Thus dopant atoms in n-type semiconductor is called donor impurity. As we observe in Fig.2.3(a) the n-type semiconductor has donor impurities their energy level located close to the conduction band. Thus electrons can jump to the conduction band by covering small energy gaps compare to in the intrinsic semiconductor. Free electrons release by donor impurity atoms in n-type semiconductor can move from the donor impurity to conduction band even at room temperature

and contributes to the conductivity.
On the other hand when trivalent dopant (B) is added to the silicon crystal semiconductor, the boron atom occupies the same position of the silicon atoms in the crystal. A trivalent dopant atom forms covalent bonds with three neighbouring semiconductor atoms as we observe in Fig.2.2b. However, dopant atom has not electron to share with the fourth neighbouring semiconductor atom. Thus we can see a hole which is created in the lattice and each trivalent dopant atoms create one hole in the crystal lattice of the semiconductor. At room temperature some electrons break away from the bonds giving the electrons to the holes phase. Simultaneously, some of the electrons recombine with the hole and reduce the number of (n_i) intrinsically generated electrons (n_e). Thus number of holes in semiconductor doped with in a trivalence dopant is much larger than number of electrons in it. If the positive charge is veiwed to be associated with a hole, thus positive charge holes act as majority charge carrier in a semiconductor doped with trivalent dopant, such extrinsic semiconductor is called p-type semiconductor. Inspite of having number of hole (n_h) greater than number of free electrons(n_e) the p-type semiconductor crystal remains neutral. As the charge to additional charge carrier is equal and opposite to that of the ionized cores in the lattice. The movement of holes as charge carriers occur when the valence electrons from neighbouring semiconductor atoms jump to fill the hole created by the dopant atoms in p-type semiconductor. When the valence electron fulls for the hole generated by the dopant, the dopant atom becomes negatively charge. Thus dopant atom in p-type semiconductor is called an accepter impurity. As we see in Fig.2.3(b) p-type semiconductor has accepter impurity energy band that located just above the valence band. Thus the free electrons can be left valence band by covering much smaller energy gap as compare to the intrinsic semiconductor. The valence electron in p-type semiconductor can move from valence band to the accepter impurity energy band even at room temperature, decrease holes in the lattice. Thus electrical conductivity of p-type semiconductor is much better than intrinsic semiconductor and hole leaves in valence band.
In general impurity diffusion in semiconductor is very important in the doping of the base materials. Understanding of the diffusion of foreign atoms is highly important because the diffusion of group III and group V elements play a vital role in the doping of the base materials of electronic devices as well as in the various thermal annealing treatments during device fabrication. On the other hand, diffusion controls the incorporation of unwanted impurity atoms [17, 18].



(a). At room temperature elctrons transfer from the donor impurity to conduction band because of the the dopants have free electrons or unpaired

(b). At room temperature the covalent bond of semiconductor becomes break down and elecrons transfer from valence band to holes (Accepter impurity).

Figure 2.3: (a). It indicates as the position of the donor impritiy(free electrons) and transfer to conduction band in its room temperature and
(b). It shows the positon of accepter impurity (holes) and the electrons transfer from the valence band to hole in its room temperature [16]

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2.2 Diffusion theories

The science of diffusion was tried to described by the earliest scientists [19]. Thomas Graham also studied the diffusion phenomenon with simple, elegant and definitive experiments that established the statement "diffusion followed a diminishing progression at longer intervals of time the mixing process decreased and that the diffusion rates in liquids are much slower than in gases". These concepts later became the bases for mathematical treatment of the diffusion process. Diffusion is material transport by atomic motion. Inhomogeneous materials can become homogeneous by diffusion and the temperature should be high enough to overcome the energy barriers to atomic motion. Theory of diffusion is now considered as ubiquitous in all three states of matter and in materials of technological interest, diffusion has assumed as great impor-tance in their design, fabrication, and performance. Diffusion in general is the redistribution of particles as a result of random (Brownian)

motion. Random motion requires that there are no any kind of driving forces. The redistribution of impurities most of the time pronunced at high temperatures and it exists in all types of matters. By understanding and controlling the diffusion has a great importance for science, technology as well as for economy. Diffusion is widely used in the electronic industry for the introduction of impurities in semiconductors in order to obtain desired changes in their electric and/or optical properties. Diffusion is the movement of particles due to concentration gradients from a region with higher concentration to a region with lower concentration, due to a thermal motion of atoms [20]. Diffusion coefficient is defined to describe the magnitude of diffusion per unit time. This coefficient is characteristic for each combination of diffusing particles and media. The definition of diffusion coefficient is given by the general equation for flux of atoms moving through a plane of unit area.

$$J(x,t) = -D(x)(\frac{\partial C(x,t)}{\partial x}) \tag{2.1}$$

This equation is known as Fick's first law, where J(x,t) is the diffusion flux measures the amount of particles that will flow through a unit area during time interval. D(x) in [cm^2/s] is the diffusion coefficient (or often called as diffusivity) and C(x,t) is the concentration of moving atoms [atoms/cm^3]. The time dependence of the concentration is given by the Fick's second law

$$\frac{\partial C}{\partial t} = \frac{\partial [D\frac{\partial C}{\partial x}]}{\partial x} \tag{2.2}$$

This is drived from the continutiy equation of $\frac{\partial C}{\partial t}$ + $\nabla .J$ = 0 assuming there is no volumetric source. If the diffusion coefficient D is constant with respect to time, the concentration in Eq.(2.2) will be reduced to position dependent form

$$\frac{\partial C}{\partial t} = D[\frac{\partial^2 C}{\partial x^2}] \tag{2.3}$$

Free charge carriers both electrons and holes can be introduced in to both inorganic and organic semiconductors by doping chemically, with impurity, illuminating with photons and injecnting from metal contact. Temperature has profound influence on the coeficient and rate of diffusion. As a result the diffusion cofficients of common impurities in semiconductor is depending exponentially on temprature [21] which is given by:

$$D = D_o exp(\frac{-E_d}{k_B T}) \tag{2.4}$$

where D_o = temperature independent pre exponential constant which is an attempt frquency proportional to frequency of atom (impurity) vibration to jump, E_d = activation energy or the energy require to jamp (diffuse) the barrier, D = the diffusion

rate (diffusivility of impurity atoms depends on exponentially on temperature upon the Arrehnuis), k_B = Boltzmann constant and T = temperature.

CHAPTER 3

The Model

We consider a three dimensional semiconductor layers with a length of 50 nm from the center to each edge. The semiconductor is extended along y and z directions and very large compared to the size along x. Let we form 101 $\times$ 101 $\times$ 101 sites along x , y and z axes. If the sample is heated the impurities ionize and then the non interacting impurities jump from one interstitial lattice site to another interstitial lattice site throuhgout the nearest neighbouring site. The sample is inserted in one dimensional external parabolic potential that varies along x dimension. Such a potential can be formed by splite gates arrangment [4, 10] thus impurities undergo a random walk assisted by one dimensional external parabolic potential which has a stable point and varies along x direction and homogeneous temperature. The device processing should take place at relatively low temperatures as quickly as possible and leaving the impurities profile relatively undisturbed. The value of position dependent external parabolic potential along the x direction which has a minimum at the center of the semiconductor layer is given by

$$V(x) = V_o X^2 \tag{3.1}$$

where V_o is the potential amplitude at the edges, X = x/x_{max}, x is a position between 0 to maximum value (L_x) or X_{max} = L_x, the value at the edge of the device along the x-axis. This means that V(x) values from 0 at the center to V_o at the edge.

When there is no applied external potential, and the internal field due to the impurity is also neglected, we consider impurity diffusion through interstitial sites of layers provided that temperature is high enough. We assume that the diffusion take places by the hopping of imputritities from any site to the neighboring sites. For this system in order to hop the impurity pass via a transition state from one equilibrium state to another equilibrium state. The transition state is at a maximum energy state known as activation energy. Thus a charged impurity must

acquire sufficient energy to overcome the potential energy barrier or activation energy. From diffusion theory the probability of hopping from site i (W_{ij}) for the impurity during the time interval dt to the nearest unoccupied site j can be written as

$$W_{ij} = D_o \exp(\frac{-E_a}{k_B T})dt \tag{3.2}$$

for k_BT $\ll E_a$ where E_a is the activation energy which is the maximum of the barrier that the system has to overcome on the way from the initial site to the next neighboring final site, k_B is Boltzmann constant, T is temperature, and D_o is the attempt frequencies to jump. The hopping probability is equal in all directions, except at the interface where the particles are perfectly reflected at the edges along x direction. But the diffusion problem is in three dimensional (3D), and can be described by a 3D Monte Carlo simulation of a number of particles hopping in a finite sized lattice with reflecting end points along x and periodic boundary conditions along y and z axes. The electric field will modify Eq.(3.2) so that the hopping probability W_{ij} between neighboring sites i and j will become

$$W_{ij} = D_o \exp(\frac{-E_a - \frac{U_{ij}}{2}}{k_B T})dt \tag{3.3}$$

where U_{ij} is the potential energy difference between lattice sites j and i. The potential enregy difference U at any site (position) X on the x axis is

$$U(x) = eV(x) + U_{int}(x) \tag{3.4}$$

where V(x) is a potential at a position x and given by Eq.(3.1), U_{int}(x) is the interaction potential energy at the specified site x, and e is the unit charge. We introduce an effective temperature dependent term dτ = $D_o \exp(\frac{-E_a}{k_B T})dt$ Eq.(3.3) as

$$W_{ij} = \exp(\frac{-U_{ij}}{2k_B T})d\tau \tag{3.5}$$

This equation shows that the probability of hopping in nonlinear field is given as a function of position in the x direction which increases the complexity to obtain an analytic solution of the diffusion problem. Due to this we have used Monte Carlo simulation approach to solve this problem.

An accurate description of the internal potential suggests that large random potentials can occur near the vicinty of a given impurities at the time of diffusion

[22]. In order to conduct electric current, materials should exist a free charge carriers. Semiconductors irrespective of their type there are no free charge carriers at a temperature approach to zero like metals. In a high temperature some electrons in the valence band transit to conduction band leaving the holes in the valence band. As a result free charge carrriers both holes and electrons can exist through inorganic semiconductors at high temperatures but this is not functional in the case of organic semiconductors because of its band gap is very large compare to a thermal energy at room temperature. However, free charge carriers can be introduced in to the both organic and inorganic semiconductors by doping chemically with impuritiy, illuminating with photons and injecting from metal contacts.

The diffusion coefficients of common impurities in semiconductors are found to depend exponetially on temperatures. Temperature has a most profound influence on the coefficient and diffusion rates. Impurity atoms utilized as dopants such as phosphorus (P), boron (B) and arsenic (As) occupy substitutional or interstitial positions where the dopant atoms can contribute free electrons or holes. In the case of donor dopants, electrons that are lost by dopants assumed to be are pushed out of the edges by external parabolic potential. During high temperature processing impurities profiles are redistributed through a process known as diffusion. The internal potential arises from non homoguneous distribution of the impurities which is calculated using poissons equation, by negleting the discrete nature of impurities.

$$\nabla^2 V_{int} = -\frac{\rho(x)}{\epsilon_o} \tag{3.6}$$

where $\rho(x)$ is the charge density and ϵ_o is the static dielectric constant of the material. We impose the boundary conditions that V_{int} = 0 and $\rho(x)$ = 0 for x $\to \infty$. We ignore the boundary effects in the x direction, the charge density is assumed to vary only with the x direction. The electronic charge has been smeared out throughout the strucuture to ensure charge neutrality of the system and allowing a physical treatment of the Poisson equation. The debye length at usual growth temperatures is much larger than the separation of minimum energy interestitial sites [23]. Therefore, we may reasonably assume that an electric field due to fluctuations in the electronic density can be neglected for the distances smaller than the Debye length [22, 24] and then the internal potential is evaluated by solving the Poisson equation. The impurities have been set to have equal diffusion constants and Arrhenuis activation energies. We aim to show the general diffusion

characteristics on the parametrs. A more detailed analysis can be performed after experiments have been performed.

The exact Monte Carlo simulation steps are
1. We place a constant number of impurities at each x site; we have chosen to place 10 impurities per site at initial at 600 K temperature and each sites represent in three dimentional (3D).
2. The potential energy differnce is calculated to observe and determine the left and right hopping probabilities for each particle.
3. Random number is generated and the probability is compared with the random number and the hopping impurity is determined based on the metropolis algorithm criteria. We repeat the steps until the impurity density profile has converged (remains stable with time). The calculation is repeated by setting different number of impurities and also for 600 K temperature.

During a device processing, there are usually many steps each at a particular temperature [10, 25]. These changes in temperature can be easily incorporated in the Monte Carlo calculation since Monte Carlo method is ease and flexible in modeling experiment. Further more processing may not last long enough for the impurities profile to reach at equilibrium, and the Monte Carlo simulation can predict with reasonable accuracy for these nonequilibrium doping profiles. In addition, further impurities can be introduced during the simulation at a specified rate that can be time dependent, to simulate impurities entering the sample from an impurity source. The time dependence of the external potential can be incorporated simply in the Monte Carlo simulation. In comparison, extending numerical techniques to include a time dependent external potential in the coupled drift diffusion and Poisson equations is not trivial.

Monte Carlo simulation Methods

Monte Carlo methods (MCM) are broad class of computational algorithm that rely on repeated random sampling to obtain a numerical results (estimation of unknown parameters). It is often used in physical and mathematical problems and are most useful when it is diffucalt (impossible) to use other approach. Many quantitative problems in science, enginee-ring and economics are now a days solved via

statistical sampling on a computer. Such Monte Carlo methods can be used in three different ways
(1) to generate random objects and processes in order to observe their behavior
(2) to estimate numerical quantities by repeated sampling and
(3) to solve complicated optimization problems through a randomized algorithms. In physics related problems, Monte Carlo methods are useful for simulating systems with many coupled degree of freedom, such like fluids, disordered materials, strongly coupled solids, cellular structures and interacting particle in systems etc. Therefore by using Monte Carlo method or techniques we can investigate and find various properties (behaviors) of impurity diffusion in semiconductors. Generally, the Monte Carlo (MC) method is known to be a versatile tool for the study of carrier transport phenomena in a large variety of semiconductor materials and devices. It is the most useful approaches to scientific computing due to its simplicity and general applicability. The next generation of Monte Carlo techniques will provide an important tools for solving ever more complex estimation and optimization problems in engineering, finance, statistics, mathematics, computer science, the physical and life sciences [26, 27]. Random numbers can be assumed as a squance which the next number in the sequence comes from the function of known an arbitrary parameters. These numbers generated by computer in this way known as pseudo random. its linear congruential random number generator is defined by the function

$$f(x, M) = X_t/M, \tag{3.7}$$

where the state X_t satisfies the linear recursion

$$X_t = (aX_{t-1} + c)\text{mod}M, \; t = 1, 2, \ldots .$$

where a, c and M are integers that are chosen. For a better pseudo random numbers the distribution should abide to draw samples usually from a uniform distribution in the interval [0,1) for a long period to be the function f is fully deterministic, at a given number x_i will generate the same to x_{i+1} next in the sequence. The advantage of this technique is that we need only sample quite a small fraction of the states of the system in order to get accurate estimates of physical quantities. When the same sequence will keep on repeating over other and reach in an equilibrium. Then we describe the simulation for calculating Coulomb interaction potential and determining impurities doping profiles.

Chapter 4
Results And Discussion

The results are presented for a one dimensional lattice since the parabolic external potential affects only the movement along the x-axis but not that along the y and z-axes. As a result we have investigated the impurity profiles only that along x-axis. It means that we have considered 101 interstitial sites in our simulation with the separation between sites fixed to 1 nm to display our results. We set the dielectric constant ϵ_o = 11.4 which is the value of silicon. The results are provided for a different values of temperatures, impurities and potential amplitudes. The electrons experience a force opposite to the direction of the movement of impurities and then impurities are free from the influence of electrons force. The calculation is done until the impurity density profiles has stabilized at a certain value of temperatures.

In Fig 4.1 we have shown the impurity distribution versus lattice sites for a constant parabolic external potential amplitude of V_o = 1 V and temperature T = 600 K for a different time steps starting from initial distribution excluding the inernal field due to impurities. At the initial of our simulation we placed dopants of density $1.96\times10^{19}cm^{-3}$. Which means 200 impurities per site at each of 101 sites along the x-axis. The number of impurities after 100, 200, 300, 400,...800 time steps were plotted. From this plot as we have observed in the figure the line in 600 and 700 time steps are over laped to each other which indicate as the impurity density profile has stabilized and reached equilibrium. As the time steps increases the impurities around the centeral region of the lattice increases untill the maximum density is attained at a time step around 600. The impurity density profile after the equilibrium has reached shows clearly that the peak is reached around the center. But after this time step there is no significant change at each site in all aspects rather than dancing around it. At small time steps the graph does not show peak at the center or becomes wide which shows that the impurities movemnet towards

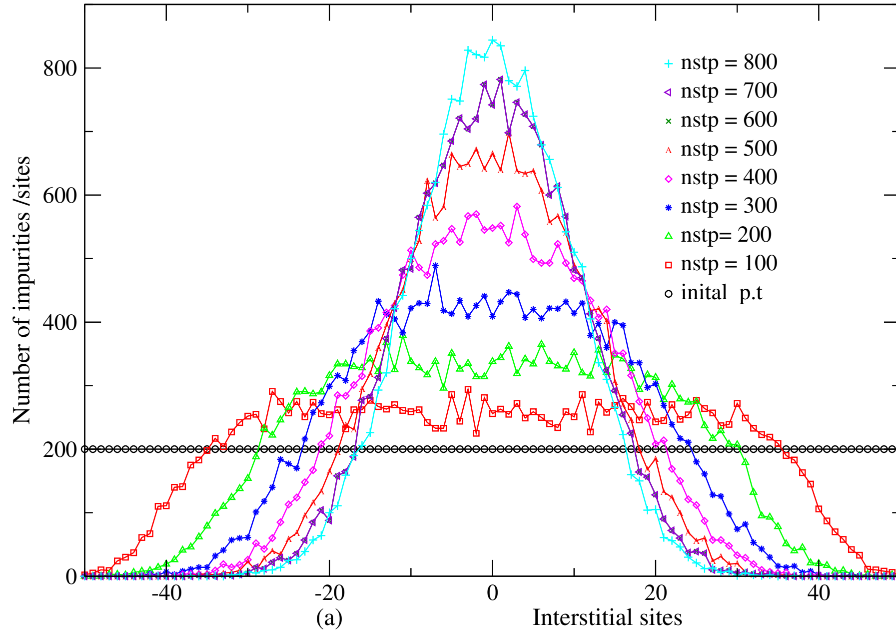

Figure 4.1: The graphs of the number of impurities at each interstitial site at initial, after 100, 200, 300,...800 time steps are shown by (circle), (square), (tringele up) (star), (diamond), (char), (cross) ,(triangle left) and (plus) respectively. The internal field V_{int} is not included in the simulation. The impuritiy density is set to $1.96 \times 10^{19} cm^{-3}$, with constant external parabolic potential amplitude (V_o) value 1 V and temperature of T = 600 K.

the center has continued. This results got due to the influence of external potential within number of steps. If the external potential change to 2 V the time step of stability also change even the temperature remains the same.

Figure 4.2 shows the plots of number of impurity distribution versus the interstitial sites similar to that in Fig.4.1 for T = 300 K as the number of the time steps increases the sharpness of the graph also increases in this case it becomes stablized for the same parabolic external potential amplitude of V_o = 1 V and the equillibrium begins from 500 time steps. This mean that the graph for 500 and 600 time steps overlap which tells us that the graph could not show any more sharpness than this point even if we increase the number of time steps. As we have seen in the graph eventhough the number of particles per sites were uniformly distributed initially that is 200; the number of impurities per site is increased around the center with the time steps until it arrived at the equilibrium, and the maximum number of impurities per site is reached after 500 time steps. At small time steps the plot does

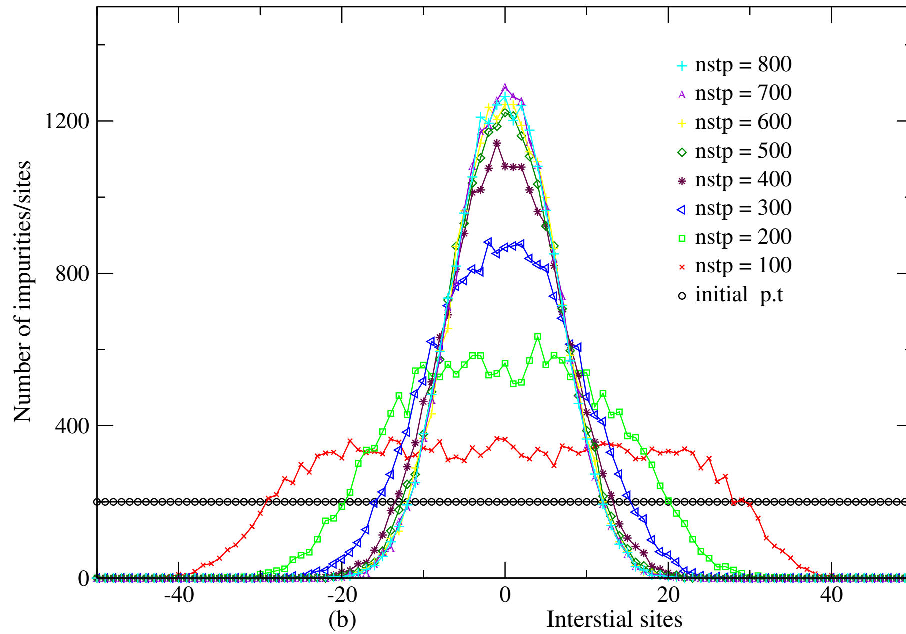

Figure 4.2: The graphs of number of impurities at each interstitial sites at constant parabolic potential amplitude V_o = 1 V and temperature of T = 300 K for different number of time steps in the simulation at inital or starting of time step, after 100, 200, 300, ..., 800 time steps are shown by (circle), (cross), (rectangle), (triangle left), (star), (diamond), (plus), (chart), and (plus) respectively with out internal field. The impurity density is set 1.96x10^{19}cm^{-3} in the simulation initially.

not exhibit a fixed peak which it indicates that the impurities still continued distribution towards the center. In general when we compare the simulation results in 600 K and 300 K temperatures we can conclude as the temperature is lowered from 600 K to 300 K the sharpness of the graph is increased, and also impurity profiles stabized more rapidly. Then number of impurities per site would be higher at the sharper point of graph in the case of 300 K temperature which indicates that the external potential influence is more pronounce when the temperature decreases. In addition to that the impurities diffusing through the interstitial site due to a temperature of 600 K is greater than the impurities diffusing through lattice (interstitial) site of 300 K temperature. It means that the impurity diffusion increases because of the diffusion in semiconductors is directly proportional to the temperature. If the value of temperatures increase the diffusivilty or movement of impurity in semiconductor also increase then impurities may not be built up at the center. It indicates that the external potential has low probability of controlling impurities diffusion in the semiconductor.

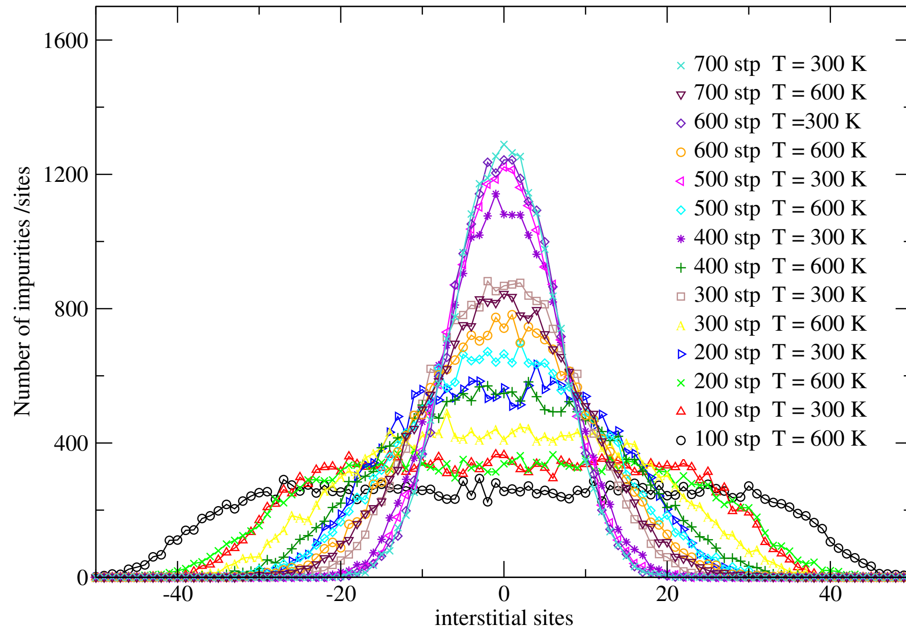

Figure 4.3: The graph of number of impurities versus lattice sites when the temperature is 300 K and 600 K during the diffusion of impurities with same external parabolic potential V_o = 1 V and number of particles (with its impurity density of 1.96x10^{19}cm^{-}3) at the common after 100, 200 ...700 time steps in the absence of internal field.

The graphs in Figure 4.3 show the effect of temperature on controlled impurities diffusion in 1 V exteranl parabolic potential amplitude with 200 number of particles per site is placed at the initial. The graphs show relatively sharp maximum at the centeral region when the temperature is lower. Thus from this graph we understand that the effect of external potential on the impurities movement is increased as the temperature is decreased. Which means that the effects of external potential becomes less when the temperature is increased and then the effect of external potential is inversely relation with temperature. This is expected as the thermal kick (k_BT) that each impurity acquires to hop over the barrier increases with temperature.

The plots in Figure 4.4 also represent the number of impurities versus interstitial sites for different temperature at constant parabolic exetrnal potential amplitude of 1 V and the same number of particles (200) or 1.96×10^{19}cm^{-3} per site at initial to understand the effect of the temperat-ure in diffusion of impurity in semiconductors after 700 time steps. Ther-efore the results shows as the impurity diffusion

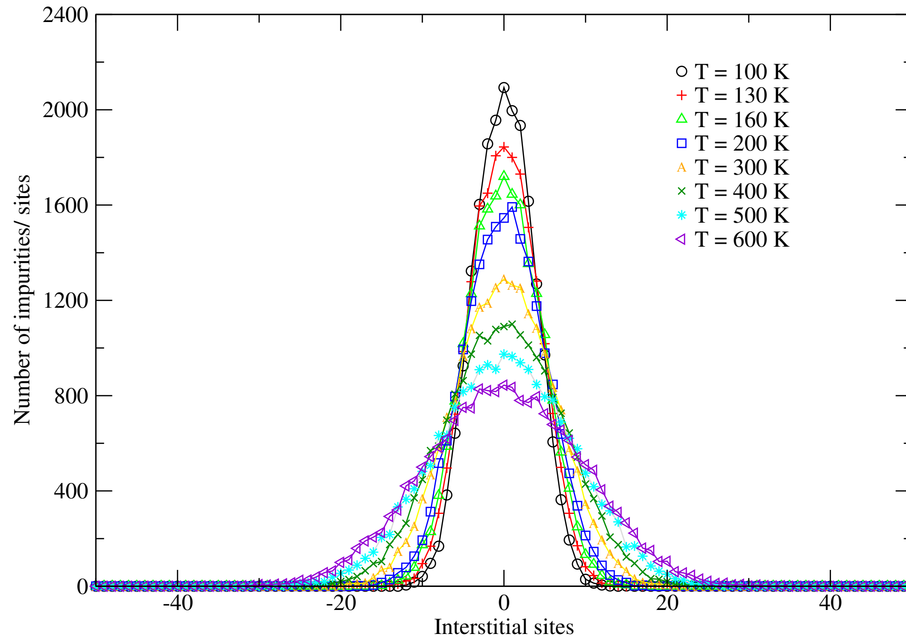

Figure 4.4: The graphs of the number of impurities versus interstitial sites after 700 time steps as a function of temprature. The plots corresponding to a T = 100 K, 130 K, 160 K, 200 K, 300 K,...600 K are indicated by (circle), (plus), (triangle up), (square), (chart), (cross), (diamond) and (triangle left) respectively at constant external parabolic potential amplitude of V_0 = 1 V and impurity density of 1.96×10^{19}cm^{-3}.

at 600 K is greater than the impurity distribution at 500 K, in a simlar case the impurity distribution at 500 K greater than diffusion of impurity at 400 K greater than diffusion of impurity in 300 K greater than impurity diffusion in 200 K and impurity diffusion in 200 K is also greater than diffusion in 160 K greater than impurity diffusion in 130 K and greater impurities distribution than at 100 K. In other expresion impurities are more confined around the center at 100 K temperature than at 130 K, 160 K, 200 K, 300 K ...600 K temperature. This indicates as the temperature increases the impurities distribution in semiconductor is also increases and vice versa. When we want to control the impurities diffusion in a semiconductor the temperature should be low because of the impurity distribution is more confined aroud the center or controlled at 100 K temperature than other of temperature including in the experimental simulation from (130 K to 600 K). As the plots show that the sharpness of the curves increases as the temperature decreases. From this we can deduce that the influence of external potential to confine the impurities around the center increases when the temperature decreases and then impurities distribution in semiconductor is controlled. But when we use high temperature impurities distribution outward of the center increase equivalentely

the sharpness of the plot decrease. This means that the effect of external potential is low to confine the impurities to wards the center.

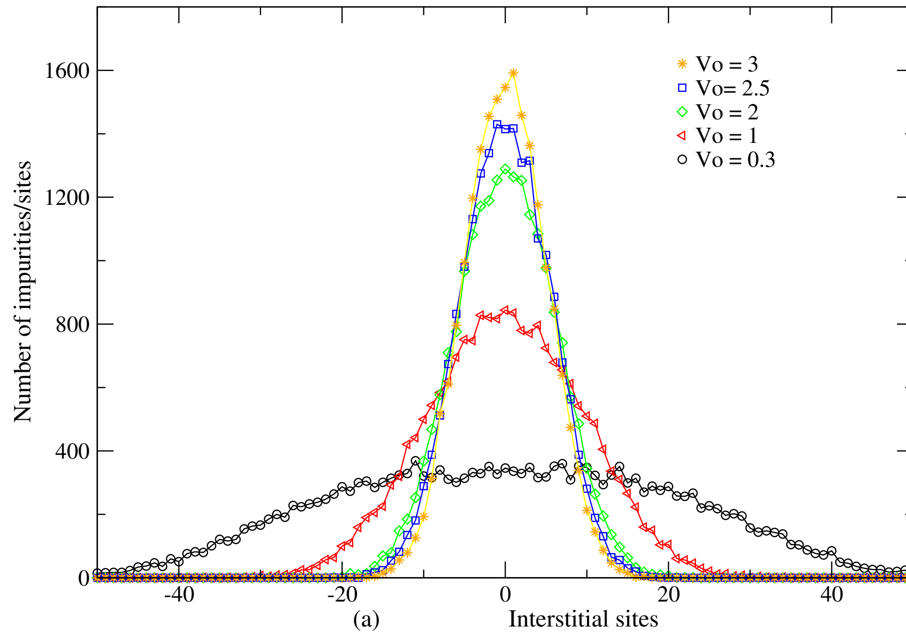

Figure 4.5: The graphs of the number of impurities at each interstitial site along x-axis after 700 time steps with the temperature of 600 K for different external parabolic potential amplitude V_o values of 0.3 V (circle), 1 V (triangle left), 2 V (diamond), 2.5 V (square) and 3 V (star) respectively. In this simulation the intial doping density is set to 1.96x10^{19}cm^{-3} per sit by excluding internal potential.

From the graph of Figure 4.5 The grahp of impurities versus interstitial sites after 700 time steps with a constant temperature of 600 K and other parameters of the impurities density of 1.96×10^{19}cm^{-3} or number of particles 200 per site initially by excluding the internal field of Monte Carlo simulation the results indicate that the sharpness of the curves for the plots increases when the external potential is increased. Which means that the external potential pushes the particles towards the center, but the temperature favors the movement (distribution) equally in all directions. Consequently the particles are more confined around the center when the external potential gets larger. As we observe on the graphs when external potential amplitude value is 0.3 V impurity diffuses or distributes through out the intersitial sites or lattice sites from -50 to 50 then the plot has large width and less sharpness. The influence of 0.3 V external potential is small to confine the particles towards the center unless the other parameter is altered. With a similar ideas

when the value of external potential is 1 V the impurities distributions covered from -30 to 30 of the intersititial sites in x-axis which is decreased the distribution related to the distribution on 0.3 V potential but it increases in the sharpness of the graph. This tells us the effect of 1 V external potential is greater than 0.3 V external potential to confine the particles profile around the center. When we consider on the value of 2 V external parabolic potential the diffusivility of impurties throughout the area of interstitial sites along x-axis decrease and covers between -20 to 20 but the sharpness of the graph is increased. Means that the probablity of impurity per sites also increase around the center. In the case of 2.5 V and 3 V values of the extrenal potential the distribution of impurities throughout the intrestitial sites at x- axis almost remains the same but the sharpenss of the graph is increased with respect to the value of external parabolic potential and the density of impurities becomes more concentrated at the center of the graph. Therefore we can conclude as the external parabolic potential increases the impurities are confined more towards the center and number of impurities per sites also increased. But the impurities distribution through out the axis of interstitial sites along x-axis decreased.

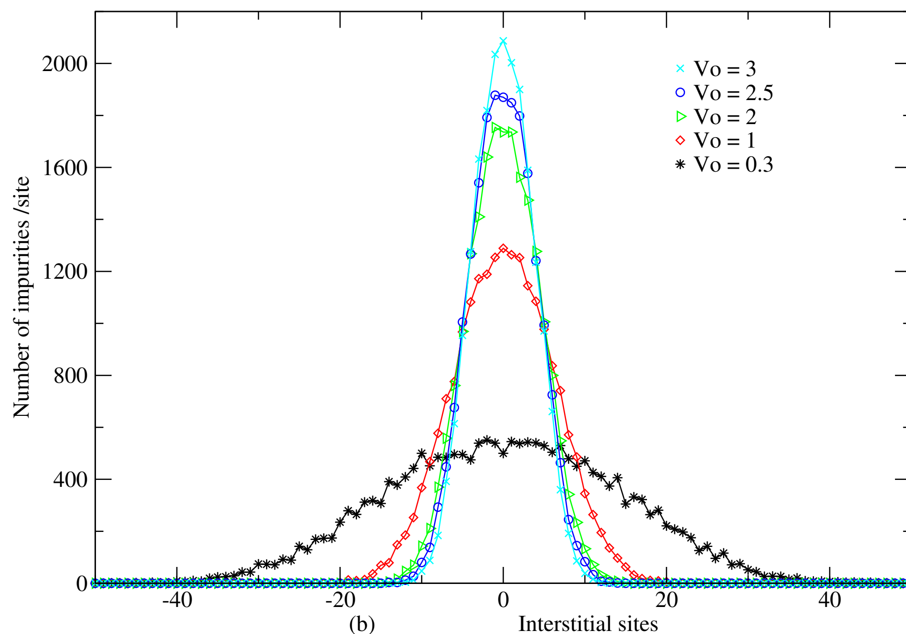

Figure 4.6: The graph of the number of impurities at each interstitial sites after 700 time steps at the temperature of 300 K for different external parabolic potential amplitudes of V_o value 0.3 V (star), 1 V (diamond), 2 V (trianle right), 2.5 V (circle) and 3 V (cross) respectively. The internal field is not included in the simulation and initially the impurity density per site is set $1.96\text{x}10^{19}\text{cm}^{-3}$.

From the graphs shown in Figure 4.6 of impurities versus lattice sites after 700 time steps at 300 K temperature. The simulation is taken with 200 number of particles per site at the initial as a function of the external parabolic potential amplitude V_o = 0.3 V, 1 V, 2 V, 2.5 V and 3 V. From this experimental results we understand that when V_o = 0.3 V the impurities are distributed through the interstitial site from -40 to 40 and impurities also try to diffuse to the center slightly. On the other hand of V_o = 1 V the impurities cover between -20 to 20 throughout the interstitial sites along x-axis shows that the confining of impurities around the center and also increased the sharpness of the graph highly relative to potential of 0.3 V. When we consider the value of external parabolic potential V_o = 2 V, the interstitial sites along x-axis they cover from -10 to 10 and the sharpness around the center increases compared to the graphs for potential amplitude 1 V. Even though the impurities distribution along the interstitial sites almost remains the same in other values of external potential, they have variation in sharpness of graphs with respect to their value of potential. Therefore we can summarize as the amplitude of external potential increases the number of impurities per site also increase around the center and decrease at the sites further from the center, and then the charges at the center will be high. This indicates that the impurity diffusion is controlled more easly. So we can use in a fabrication industries and laboratories to control what unwanted charges or impurities.

As we have shown Figure 4.7 of number of impurities versus interestitial sites after 700 time steps with 200 initial number of particles per site to compare the effect of temperatures of 300 K and 600 K on external parabolic potential functions and then to determine the impurity profiles. The plots in 600 K temperature along x-axis are wider than plots in 300 K temperature in the same external parabolic potential amplitude. This means that the sharpness of the curves in the graphs of 600 K temperature are lower than curves of graph at 300 K temperature. Equally the impurities profile per site at 300 K temperature are higher than at 600 K temperature. These indicate that at 300 K temperature the external potentials are more effective to confine the impurities (particles) around the center than at 600 K temperature.

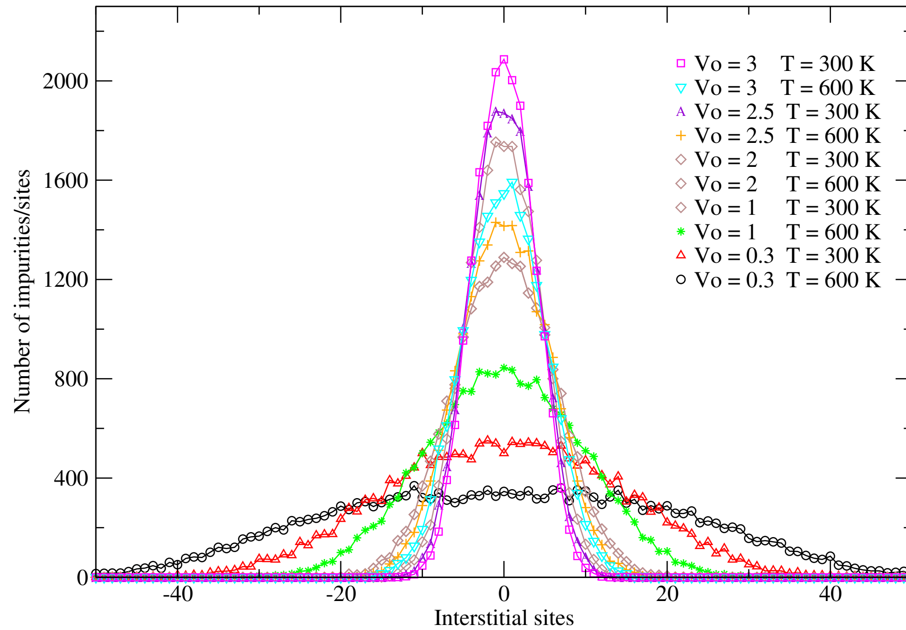

Figure 4.7: The graphs of the number of impurities versus interestitial sites along x-axis after 700 time steps with 200 number of particles per site for different external potential to compare the effect of external parabolic potential amplitude in 300 K and 600 K tempratures in the absence of Coulomb interaction in the simulation.

The plots in Fig 4.8(a) show a number of impurities versus interstitial sites at constant potential amplitude V_o = 1 V when the temperature is (T = 600 K) for different numebr of impurities 10, 50, 100 and 200. The resuals indicate that the deffusivility of impurity increases with density or the diffusivility of impurity is directly proprtional to the density or numbers of particles at each sites becomes increased around the centeral region. In similar case when the temperature is 300 K but others remain constant, and the density increases the diffusivility of impurity also increases and the number of impurities per site around the center also increase. But degree of diffusivity of impurity is different at temperature of 600 K and 300 K. Because as temperature steps up the diffusivility increase and modify the sharpness of the graph which becomes less and then becomes wider than the graphs at temperature of 300 K. Therefore, we can generalize that the diffusion of impurtiy in a semiconductor increases when the number of particles in each sites (dopant density) increases keeping other parameter such like external parabolic potential and temperature constant. Similarly at constant external potential and doping density, the diffusion of impurtiy increases with increasing tempe-rature. So, the shape of impurities profile in semiconductors can be determined based on

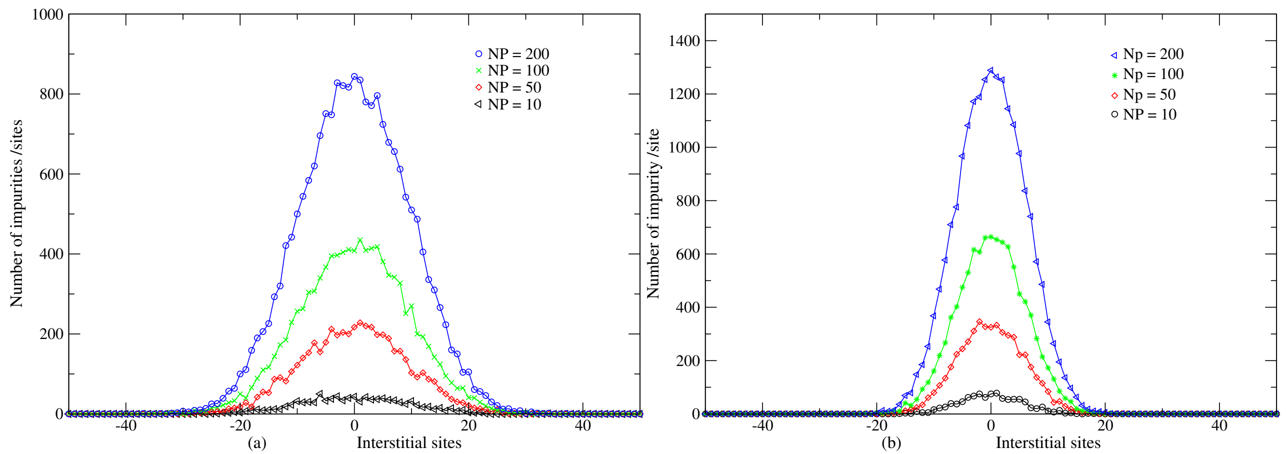

Figure 4.8: (a). The graph of number of impurities at each interstitial sites at constant external potential amplitude of (V_o = 1 V) and temperature of T = 600 K as a function of dopants density (number of particles) per site of (triangle left) (9.81x$10^{17}cm^{-3}$), (diamond) (4.9x$10^{18}cm^{-3}$), (star) (9.8x$10^{18}cm^{-3}$) and (circle) (1.96x$10^{19}cm^{-3}$).
(b). The graph of number of impurities at each interstitial sites with the external potential amplitude of 1 V with a temperature of T = 300 K as a function of impurities density or number of particles per site of (circle), (diamon), (star) and (triangle left).

temperature, external potential and doping density.

The graphs in Fig.(4.9) show the impurities profiles after 700 time steps for different number of particles and temperatures. As we observe in the figure a graph has more sharpness at 300 K temperature than at 600 K temperature provided that number of particles initially placed at each site is same. This tell us the impurities density is increased with a sharpness of the graphs. The diffusivity of impurities towards the edge becomes low as the temperature decreased .

The graphs in Fig.(4.10) show the impurities profiles after different time steps for external parabolic potential V_o = 1 V, temperature T = 600 K and 200 number of impurities per site is set initially in the presence of internal field. We understand that as the time steps increases the number of impurities per site also increase until it attained stable in 800 time steps because of 800 and 900 time steps overlap. The point of the equilibrium attains slowly compare to in the absence of internal field. The other understaning from these graphs when we include the internal field (Coulomb interaction) the point of equilibrium steps up to 800 time steps compared

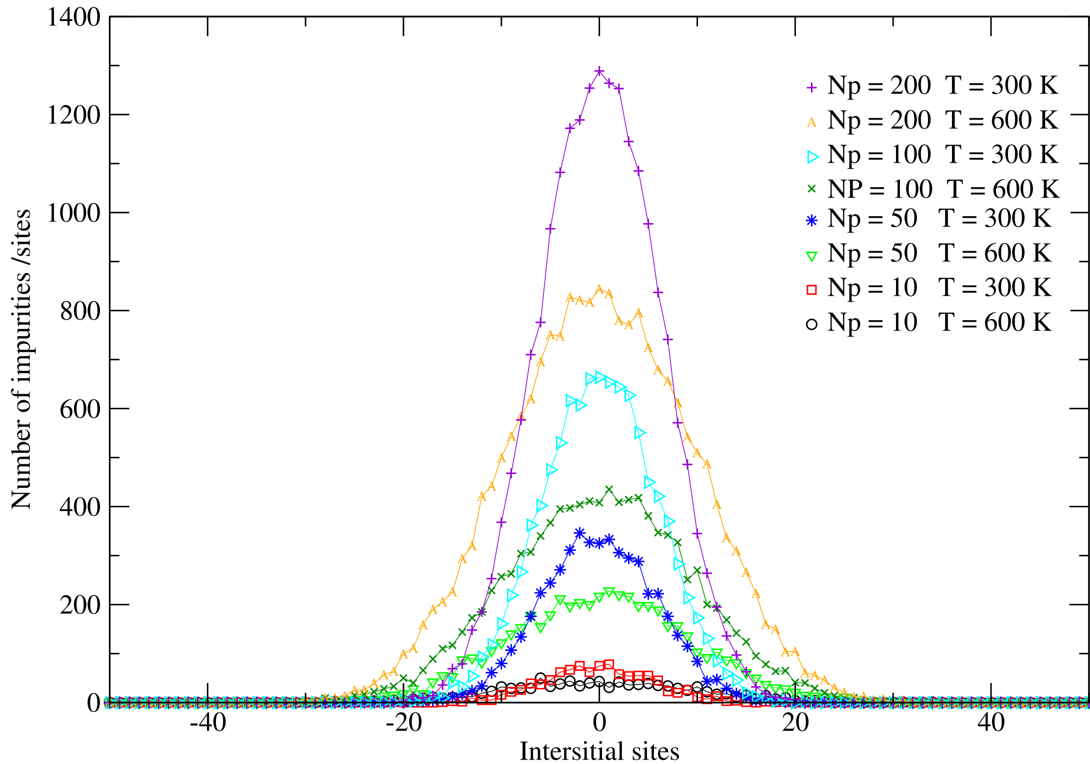

Figure 4.9: Graphs of number of impurities versus interstitial sites after 700 time steps at different dopant density when the external potential amplitude is 1 V to compare effect of temperature in a number of impurities.

to point of equilibrium 700 time steps in the absence of internal field as it described in Fig.4.1. Eventhough the point of stability of graph in the persence of internal field increases,there is no significant change in the width of the graphs along x-axis. This indicates that the internal potential try to push particles to all direction of semiconductor contary to the influence of external potential but not more effective. So, we can generalize that the internal potential and temperaure effects are opposite the effect of external potential of confined particles around the center but the influence of internal field may be small and then no significant change along the width.

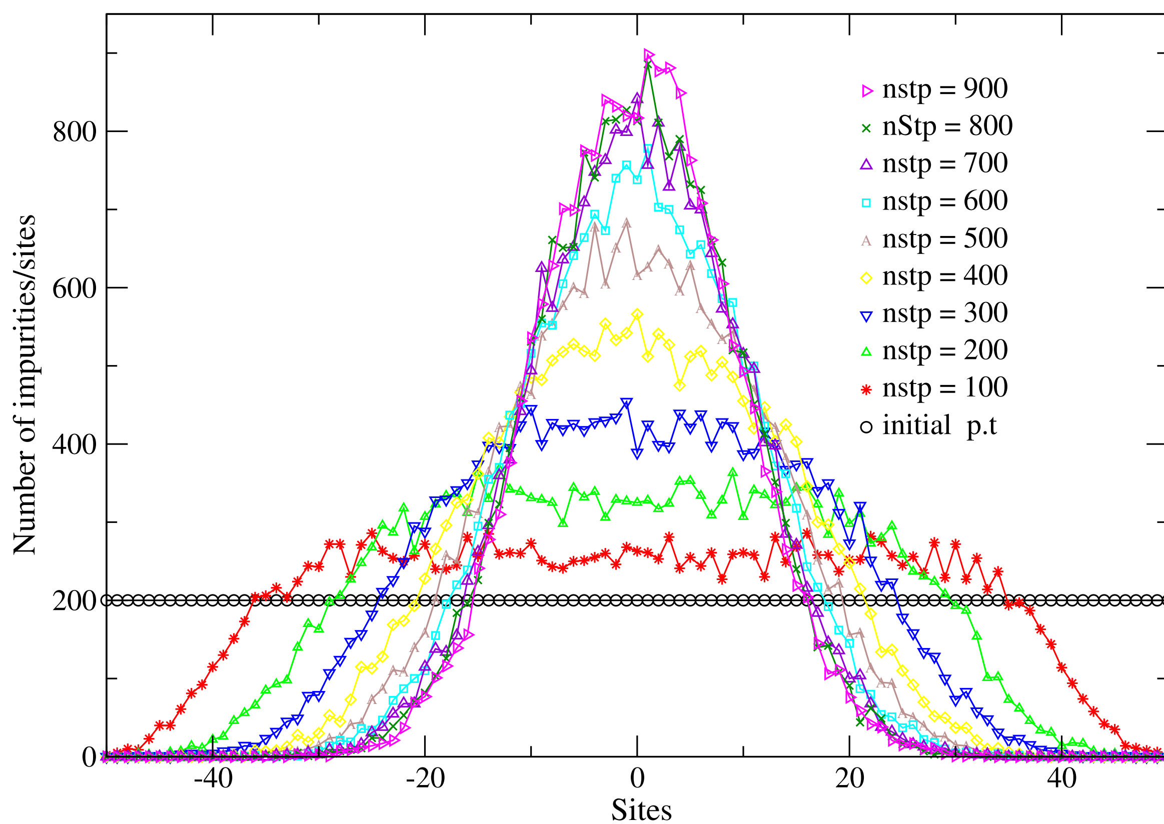

Figure 4.10: The graph of number of impurities versus the interstitial sites at T = 600 K and external potential of V_o = 1 V including the Coulombs interaction in simulation at dopant density of $(1.96\times10^{19}cm^{-3})$ is set initially in the simulation for different time steps.

CHAPTER 5

Summary and Conclusion

Semiconductors were viewed as a solids with irreproducible properties. but now the Scientific efforts overcame this idiosyncrasy and turned the art of impurity doping into versatile useful and repreducable technology applications. Proper understaning of the fundamental physics of impurities diffusion in a semiconductor has great significance for technology to create impurity profiles that used for electronics and fabrication of many devices that are important for the constructions of modern electronic equipments. Impurities are usually introduced at high temperature by the technique of ion implantation and diffusion since they controlled number of impurity atoms that can be introduced in to a specific regions of the crystal. But compare to method of thermal impurity diffusion (forced impurity diffusion) technique, ion implantation has structural defects that are difficalt to cure. The conductivity of semiconductors can be manipulated by varying the concentration of impurities and the background of temperatures. As a temperature and concentration of semiconductor increased its conductivity also increased. Thus the diffusivility of dopants increase as the dopants density increase and then the location of the high density region is linked to the shape of the external field. The conductivity of semiconductor is increased either at high temperature or by introducing impurities to it.

In this paper we have performed a three dimensional (3D) Monte Carlo simulation to evalute and determine the impurity profiles and controlled impurity distribution by the help of external parabolic potential amplitude and temperatures. We assumed as the simulations are performed well in the ionized impurities which diffuses by the interstitial mechanism. Because the interstitial mechanism has very low activiation energy, fast and very smaller characterstics than other diffusion mechanisms. The internal field is calculated in the simulation without considering the discrete nature of charge distribution. The probability of occuring the internal field is increased with the increasing of dopant density and temperatures that

causes broadening of the plots after certain critical doping density and temperature. The internal field becomes significant and normalize the effect of external potential. Similar to that in our system we expect as it resists the accumulation of charges around the center by the external potential. If the effect of the internal potential in the system is very small, the impurities profile accumulated by external field may not be influenced rather than alters the point of time steps of stability.

The width of impurities profiles can be controlled by the curvature of parabola, which is the curvature of barabola becomes sharp when the external parabolic potential amplitude increased but the temperature becomes decreased. On the other hand the curvature of parabola is broaden when the number of impurities (density) becomes increased equally the temperatures increased. Therefore, we can be generalize as the presence of high dopant density and large coulomb interaction have great significant role of broadening the doped layer by normalizing the effect of external potential and low temperature by resist the building up of charges at the center of the system. All these points were found in this work.

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DECLARATION

I, hereby, declare that this Master of Science thesis is my original work and it has not been presented for a degree in any other university and that all source of materials used for the thesis have been duly acknowledged.

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