Chapter 2

Range profile, Energy loss and Damage distribution for ion-solid interaction

2.1 Range profile and Energy loss

2.1.1 Introduction

The depth at which the implanted ions come to rest in the solid depends on the interaction of ions with electrons and nuclei and the consequent energy loss. A knowledge of this penetration depth is important for the fabrication of a doped or modified layer in a substrate by ion implantation. The versatility of ion implantation can be exploited only after a detailed understanding of the range profiles of the implanted ions.

An energetic ion, upon entering a target, gradually loses its kinetic energy through interactions with electrons and atoms of the target material and slows down to rest. The mechanism of energy loss can be distinguished into:

• (1) Nuclear collisions, in which the energy can be transferred from the nucleus of the projectile to that of a target atom by electrostatic interaction between the screened charges of the two nuclei. This nuclear energy loss, as it is usually
called, may be viewed as an elastic interaction between two free particles.

- (2) Electronic collisions, in which the moving particle excites or ejects atomic electrons. This electronic energy loss comes from the "frictional resistance" that the projectile encounters on its passage through the electron clouds surrounding each target atom, and is viewed as an inelastic interaction due to the complex nature of the energy loss process.

For most purposes, this separation into elastic (nuclear energy loss) and inelastic (electronic energy loss) collisions, although not strictly valid, is convenient and is a good approximation. The first type of collision can involve large discrete energy losses and significant angular deflection of the ion trajectory, whereas second type involves much smaller energy losses per collision, negligible deflection of the ions and negligible lattice damage. However, the electronic slowing down mechanism also introduces statistical energy straggling in an initially mono-energetic ion beam. The relative importance of the two energy-loss mechanisms depend on the energy of the ion and the atomic numbers of the ion-atom combination. A typical distribution of the nuclear and electronic energy loses during MeV implantation is shown in Fig 2.1. It is observed that:

- there is a high linear density of the energy contribution by ions into the electronic subsystem of the sample (electronic energy losses), amounting to tens of keV/nm.

- a small fraction (within a few percent) of the initial ion energy $E_0$ transmitted directly to the nuclear subsystem of a sample (nuclear energy losses) predominantly at the end of the mean projected range $R_p$.

The total distance traveled by the ion before coming to rest is called the range ($R$) and is given by [1]:

$$ R = \int_0^{E_0} \left( \frac{dE}{dx} \right)^{-1} dE $$

(2.1)

where $E$ is the ion energy, $E_0$ being its value at the target surface, $x$ is the distance measured along the ion path and $(dE/dx)$ is the energy loss per unit length. The
length of the projection of the ion path on its incident direction is called the projected range $R_p$. In ion implantation studies one is actually interested in the entire ion distribution as a function of depth and therefore information about the range straggling is necessary. In the absence of channeling and for ions of moderate energies, this distribution is approximately Gaussian in shape and so can be described by a single extra parameter, namely, the fluctuation (standard deviation) $\Delta R_p$ in the projected range along the direction of $R_p$. $\Delta R_p$ is called longitudinal straggling and fluctuation along the direction perpendicular to this is known as transverse straggling $\Delta R_t$. The parameters $R_p, \Delta R_p$ and $\Delta R_t$ are, in general, of great interest as a reliable description of these parameters is important for device design and modeling, as well as process optimization and control in the device fabrication environment. These are schematically shown in Fig 2.2. Quantities $\Delta R_p$ and $\Delta R_t$ have been measured in this thesis by applying the technique of tilt angle implantation.
Fig. 2.2. Projected range $R_p$ and the distribution of the implanted atoms $\Delta R_p$ and $\Delta R_t$. Also shown is the range $R$ of the ions.

2.1.2 Range-Energy Theory

The range of an ion is obtained by integration of specific energy loss, \(dE/dx\) as mentioned in Eqn. 2.1. \([dE/dx\) contains both nuclear and electronic energy loss.]

\[
R(E_0) = \int_0^{E_0} \left(\frac{dE}{dx}\right)^{-1} dE
\]  \hspace{1cm} (2.2)

where the upper bound of integration $E_0$ is the energy of the incident ion.

The corresponding range straggling ($\Delta R$) is the average fluctuation in range and is given by

\[
(\Delta R)^2 = \int_0^{E_0} N\Omega^2(E)dE \left(\frac{dE}{dx}\right)^3
\]  \hspace{1cm} (2.3)

where $\Omega^2(E) = (\Delta E)^2/Ndx$ and $(\Delta E)$ is the average fluctuation \([2]\) in the energy loss. $N$ denotes the number of scattering centers per unit volume.

As we have indicated, there are two major processes which need to be considered in developing a suitable range-energy relationship: (a) screened Coulomb collisions between the moving ion and the target atoms (nuclear stopping), and (b) interactions
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between the electrons associated with the moving ion and the various electrons (both bound and free) in the solid (electronic stopping). The basic principles governing both these processes were first stated by Bohr [2]. Later, Lindhard and his collaborators (Scharff and Schiott) [3, 4] developed these ideas into a comprehensive unified theory of atomic stopping. This theory (referred to as LSS subsequently) has been the framework and reference point for ion range theory and experiments since its inception. The theory uses the concept of the separation of elastic and inelastic energy loss, with a Thomas-Fermi potential for the elastic and an electron gas stopping power for the inelastic energy loss proportional to the square root of the ion energy.

If a universal inter-atomic potential for two colliding atoms can be formulated, the calculation of range parameters for any system would be straightforward, be it by exact numerical computation or approximate analytic expressions. By using a differential scattering cross-section based on a Thomas-Fermi potential, \( V(r) = \left( Z_1 Z_2 e^2 a^{a-1/2} r^s \right) \) where \( Z_1 \) and \( Z_2 \) denote the atomic number of the projectile and the atoms in the target medium respectively. \( s \) denotes the power of the potential and \( a \) the screening parameter in terms of the first Bohr radius \( a_0 \) and is given by

\[
a = \frac{0.8854a_0}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}}
\]  

(2.4)

\( e \) is the electronic charge.] LSS have derived a universal relationship for the nuclear stopping \( (d\varepsilon/d\rho)_n \) in terms of dimensionless length and energy parameters, \( \rho \) and \( \varepsilon \), defined as

\[
\rho = 4\pi a^2 N \frac{M_1 M_2}{(M_1 + M_2)^2} R
\]  

(2.5)

and

\[
\varepsilon = E \frac{a M_2}{Z_1 Z_2 e^2 (M_1 + M_2)}
\]  

(2.6)

\( N \) is the number of atoms per unit volume, \( M_1 \) and \( M_2 \) are the mass of the projectile and target atoms, respectively. The resulting universal relationship between \( (d\varepsilon/d\rho)_n \) and \( \varepsilon^{1/2} \) (based on Lindhard et al. [3]) is shown by the solid line in Fig 2.3 (\( \varepsilon^{1/2} \) is proportional to ion velocity).

To obtain the stopping contribution due to electronic collisions, LSS have derived
Theoretical stopping cross-section in \( \rho - \epsilon \) variables. The abscissa is \( \epsilon^{1/2} \), i.e., proportional to ion velocity. The full-drawn curve is \((de/d\rho)_n\), i.e., \( S_n \). The dashed line is the electronic stopping cross-section \( (S_e)_e \), for \( k = 0.15 \). See the text for details.

A velocity-proportional electronic stopping \((de/d\rho)_e\) given by

\[
(d\epsilon/d\rho)_e = k\epsilon^{1/2}
\]

where

\[
k = \zeta_e \frac{0.0793Z_1^{1/2}Z_2^{1/2}(M_1 + M_2)^{3/2}}{(Z_1^{2/3} + Z_2^{2/3})^{3/4}M_1^{3/2}M_2^{3/2}}
\]

and \( \zeta_e \approx Z_1^{1/6} \). The value of \( k \) is normally of the order of 0.1 to 0.2, and only in the exceptional case of \( Z_1 \ll Z_2 \) can \( k \) become larger than unity. The electronic-stopping calculations therefore do not produce a universal \((de/d\rho)_e\) curve, but rather a set of curves each characterized by a particular value of \( k \). As an example, the electronic stopping cross-section for \( k = 0.15 \) is also shown in Fig. 2.3.

To obtain a range-energy relationship from these nuclear and electronic stopping cross-sections, LSS theory treats the two forms of energy losses as being independent of each other as a first approximation; hence the overall stopping cross-section \((de/d\rho)_{\text{total}}\) is obtained by adding the approximate \((de/d\rho)_e\) curve for electronic stopping to the universal curve \((de/d\rho)_n\) for nuclear stopping as

\[
(d\epsilon/d\rho)_{\text{total}} = (d\epsilon/d\rho)_n + k\epsilon^{1/2}
\]
For an ion entering into a medium, this can be integrated from the starting energy down to zero to give the range as a function of energy. Fig. 2.4 shows the resulting $\rho$ versus $\epsilon$ relationship as given by LSS theory for different values of $k$.

The range of an ion, calculated by integrating the basic LSS stopping cross-section curves in Fig. 2.3, is the total distance $R$ that the ion travels before coming to rest. In ion implantation, it is the projection $R_p$ of this total path length along the direction of incidence that is of interest. LSS theory gives the relationship between $R$ and $R_p$ for $M_1 > M_2$ as

$$\frac{R}{R_p} = \frac{\rho}{\rho_p} \approx 1 + \frac{M_2 s^2}{4M_1(2s - 1)}$$  

(2.10)

where all the symbols have their usual meaning as stated before. $\rho_p$ is the projected length. Calculation of range parameters [5, 6, 7, 8] demonstrate that a universal description in reduced units with the scaling of a Thomas-Fermi atom is valid; the Thomas-Fermi potential, however, should be replaced by a more realistic form.
2.1.3 Monte-Carlo Calculation of Range Distributions (TRIM)

Computer simulation of the slowing down and scattering of energetic ions in materials has been performed using TRIM (transport of ions in matter)-code which has proved to be very useful in studies involving ion implantation, radiation damage, sputtering, and the reflection and transmission of ions [9]. The formalism for the TRIM-code is based on the basic principle of LSS theory i.e., the nuclear and electronic energy losses or stopping powers are assumed to be independent. Using the Monte-Carlo technique, TRIM was developed for determining ion range, damage distributions as well as angular and energy distributions of backscattered and transmitted ions. The Monte-Carlo method has a number of distinct advantages over analytical formulations based on transport theory. It allows more rigorous treatment of elastic scattering, explicit consideration of surfaces and interfaces, and easy determination of energy and angular distributions. In the simulation, the method consists of following trajectories of a large number of individual ions or particles in a target. Each trajectory begins with a given energy, position and direction. As a result of binary nuclear collisions, the particle is assumed to change the direction and move in straight free-flight-paths between collisions. The energy is reduced as a result of nuclear and electronic energy losses, and trajectory is terminated either when the energy drops below a pre-specified value or when the position of the particle is outside the target. The target is considered amorphous with atoms at random locations. This method is applicable to a wide range of incident energies, approximately 0.1 keV to several MeV, depending on the masses involved. The lower limit is due to the inclusion of binary collisions only, while the upper limit results from the neglect of relativistic effects. Nuclear reactions are not included. The efficiency for dealing with high energy particles has been increased by incorporating an energy dependent free-flight-path. Further, the nuclear ($S_n$) and the electronic ($S_e$) energy losses or stopping cross-sections are assumed to be independent of each other so that the total stopping cross-section ($S_t$) is simply additive, i.e. $S_t = S_n + S_e$. Thus, particles lose energy continuously from electronic interactions and in discrete amounts in nuclear collisions. Finally, the range parameters are obtained from the total energy loss and the calculations based on transport theory [1]. The detailed calculations for the ion range profiles (such as
total ion range, projected range, longitudinal and transverse straggling etc.) may be found in Ref. [1].

2.2 Damage Distribution

2.2.1 Introduction

During ion implantation, interactions of the energetic ion with the host atoms produce collisions. In these collisions, sufficient energy may be transferred from the ion to displace the host atom from its lattice site. The displaced atom can in turn displace other atoms, and so on - thus creating a cascade of atomic collisions within the solid. This leads to a distribution of vacancies, interstitial atoms, and other types of lattice disorder in the region around the ion track. As the number of ions incident on a crystal increases, the individual disordered regions begin to overlap. At some stage an amorphous layer may form. The total amount of damage and its depth distribution will depend on the implanted species, its energy and ion dose, substrate temperature, and the channeling effects.

An accurate knowledge of the damage profile created by ion implantation is important for a variety of reasons. In ion implantation technology the annealing of defects formed during implantation depends on the nature and density of the damage. In addition, the post-anneal lattice location of the implanted ion is a complex function of the type and degree of the surrounding disorder. Thus to understand and interpret the results of the implantation and annealing processes, a knowledge of the damage distribution is required. Moreover, knowledge of depth dependent damage in addition to substitution fraction of dopant species is essential for device fabrication.

2.2.2 Dechanneling due to lattice disorder

Rutherford backscattering spectroscopy (RBS) of energetic light ions in combination with channeling technique is a useful tool in the investigation of the lattice disorder due to ion bombardment of single crystals. The channeling spectrum contains information on the depth distribution of the damage and can be used to extract the full
depth profile of the lattice disorder. The problem can be described in the following way: At a specific depth in the crystal, the probing beam consists of a channeled component and a non-channeled component. In a perfect (defect-free) crystal, it can be possible that once channeled the particles remain in channeling trajectories. However, the channeled particles undergo many small angle scattering events with electrons. The angle with which the channeled particles cross the center of the channel slowly increases because of this multiple scattering and thus an increasing number of particles come closer to the rows and planes. Such particles can then collide with lattice atoms displaced out from their static rest positions because of thermal vibrations. The combination of multiple scattering by electrons and thermally displaced atoms at the channel walls leads to an increase, with depth, of the number of non-channeled particles. In a crystal having defects, the channeled particles scatter not only from atoms on normal lattice sites, but it may also backscatter from defects within the channel. The interaction of the channeled particles with defects can result in small angle collisions that deflect particles out of the channel and gradually increase the non-channeled or dechanneled component of the beam. The non-channeled component can undergo large angle scattering with all the atoms in the crystal. Thus, in crystals with defects, an increase in scattering yield over and above that of an ideal (defect-free) crystal can occur due to two reasons [10]:

- (1) the direct scattering of the channeled beam from defect atoms directly in the path of channeled ions, and
- (2) the gradual increase with depth in the non-channeled component of the beam due to the defect-dechanneling mechanism.

Thus, it is necessary to calculate the dechanneling contribution due to lattice disorder from the RBS/C spectra in order to obtain the depth dependent damage density. In the present thesis, the depth dependent damage density has been extracted from RBS/C experiments on MeV implanted Sb in Si for various fluences, annealing conditions and geometry.
2.2.3 Formalism

A. Energy to Depth Conversion:

In RBS/C measurement, the channeled and random particles have different stopping powers. At keV energies, for depths of less than one micrometer, the energy spreading due to stopping power difference between channeled and non-channeled particles is smaller than the detector resolution and the energy scales of both random and aligned spectra can be converted to depth scales on the basis of a one-to-one relationship. For MeV ion implantation, the energy spreading is larger than the detector resolution. Thus the one-to-one scale conversion is not valid and energy spreading between random and channeled particles must be taken into account [11]. The energy dependence of stopping power must also be considered in the depth scale conversion [12]. The width $\Delta x_i$ of each channel in the RBS spectrum varies with the depth $x$ and the stopping power ratio $\alpha$. It can be calculated as follows:

$$\Delta x_i = \frac{(K E_{i}(in) - E_{i}(out))}{[S]}$$

(2.11)

where

$$[S] = \alpha K \frac{dE}{dx} \bigg|_{EC_{i}(in)} + \frac{1}{Cos \theta} \frac{dE}{dx} \bigg|_{EC_{i}(out)}$$

(2.12)

$$EC_{i}(in) = EC_{i-1}(in) - \Delta x_i \frac{dE}{dx} \bigg|_{EC_{i-1}(in)}$$

(2.13)

$$ER_{i}(in) = ER_{i-1}(in) - \Delta x_i \frac{dE}{dx} \bigg|_{ER_{i-1}(in)}$$

(2.14)

$$E_{i}(out) = E_{i-1}(out) + \Delta x_i \frac{1}{Cos \theta} \frac{dE}{dx} \bigg|_{E_{i-1}(out)}$$

(2.15)

$$Cor_i = \left( \frac{EC_{i}(in)}{ER_{i}(in)} \right)^2$$

(2.16)

where $K$ is the kinematic factor of the host atom (Si $= 0.584$), $EC_{i}(in)$ is the channeled He$^+$ ion energy before scattering at the front of $\Delta x_i$, $E_{i}(out)$ is the energy of He$^+$ ion backscattered from the back of $\Delta x_i$. The stopping power $dE/dx$ can be calculated
from a polynomial function of energy [13] or taken from the TRIM simulation results [9]. We have utilized the results from TRIM in our study. \( \alpha \) is the stopping power ratio of the incident He ion in channeling direction compared to the random direction. It is dependent on both, channeling He\(^+\) ion energies and damage concentration [14]. In this thesis work, a stopping power ratio of 0.7 has been considered [11]. \( ERhosts\) is the energy of random particles before scattering at the front of \( \Delta x_i \). The difference between \( ERhosts\) and \( EC\) is the energy spreading; it will become larger at deeper region. Since the scattering cross section is inversely proportional to energy squared (\( \sigma \propto E^{-2} \)) [13], the influence of energy spreading on scattering cross-section needs to be considered.

In this thesis, all the energy spectra were converted to depth scales using equations 2.11 to 2.16. The yield (Y) in the RBS/C spectrum i.e. the number of counts in a channel generated by particles which are scattered within the target at an energy \( E, \) and which emerge from the target with energy \( E_1, \) can be written as [15]:

\[
Y(E_1) = Q\sigma(E)\Omega \frac{DE}{\epsilon(E)} \frac{\epsilon(KE)}{\epsilon(E_1)}
\]

(2.17)

where \( Q \) is the total number of projectiles incident on the target, \( \sigma \) is the scattering cross section, \( \Omega \) is the solid angle of the detector, \( \epsilon \) is the stopping cross section and \( DE \) is the energy width of one channel in the spectrum. According to Eq. 2.17, the aligned spectra yield \( Y(EC\)hosts) can be corrected as \( Y'(EC\)hosts) after considering the influence of energy spreading,

\[
Y'(EC\)hosts) = Y(EC\)hosts) \times Cor \frac{\epsilon(ERhosts)}{\epsilon(EC\)hosts)} \frac{\epsilon(K * EC\)hosts)}{\epsilon(K * ERhosts)}
\]

(2.18)

Therefore, the one-to-one relationship is available in the depth spectra.

B. Dechanneling Analysis:

For disorder analysis we treat the beam in the crystal at depth \( x \) as composed of two components (Fig 2.5): the 'channeled' fraction and a 'random' fraction. The random fraction \( \chi_r \) is that component of the beam that has the same scattering yield as for
Fig. 2.5. Schematic showing channeled fraction \((1 − \chi_r)\) and the random fraction \((\chi_r)\) (randomly interacting non-channeling particles) of the beam in a crystal.

A beam of particles impinging on a solid with a non-ordered or random arrangement of atoms. The random component at a depth \(x\) consists of those particles that are initially non-channeled and those that are initially channeled but are dechanneled during their penetration to a depth \(x\).

The presence of defects or disorder, \(N_d(x)\), leads to an increase in the random fraction \(\chi_r\) of the beam. In this formalism, we compare the measured channeling/backscattering yield as a function of depth to that from a defect-free (virgin) crystal, whose random fraction is denoted as \(\chi_v(x)\). The \(\chi_v(0) = \chi_{\text{min}}\), whereas \(\chi_v(x)\) includes the fraction initially not channeled, \(\chi_{\text{min}}\), and that relatively small fraction dechanneled by finite scattering interactions in the virgin crystal.

The quantity \(\chi_v(x)\) in a virgin crystal is directly measurable in a RBS/C experiment. It is often called the normalized or aligned yield and is extracted by taking the ratio of the aligned to the random yield at the corresponding depth. The corresponding quantity, the aligned yield, for a crystal containing defects is denoted \(\chi_d(x)\) and is also a measured quantity. The relationship between \(\chi_d(x)\) and the random fraction of the beam \(\chi_r(x)\) may be written as:

\[
\chi_d(x) = \chi_r(x) + (1 − \chi_r(x)) \left( \frac{N_d(x)}{N} \right) \tag{2.19}
\]

where \(N_d\) and \(N\) are the numbers of displaced atoms and host atoms in the unit volume at depth \(x\), respectively. Equation 2.19 simply states that the normalized yield in a crystal containing defects is the sum of the contributions from the scattering of the random component, \([\chi_r(x)]\), with all atoms, and the contribution of the scattering from the channeled component \([1 − \chi_r(x)]\) with defect atoms within the channel. If
$\chi_r(x)$ is known, $N_d(x)$ is easily extracted. However, $\chi_r(x)$ is not a directly measurable quantity. $\chi_r(x)$ may be estimated under two different assumptions of dechanneling mechanisms: single scattering [16] and multiple scattering [17]. For single scattering, 

$$\chi_r(x) = 1 - [1 - \chi_v(x)] \exp^{-\gamma(x)}$$  \hspace{1cm} (2.20)

and

$$\gamma(x) = \frac{\pi Z_1^2 Z_2^2 e^4}{E^2 \psi_c^2(x)} \int_0^x N_d(x) dx$$  \hspace{1cm} (2.21)

where $Z_1$ and $Z_2$ are the atomic numbers of the projectile and target atoms respectively, $e$ is the electronic charge and $E$ the energy of the projectile ions. $\psi_c(x)$ is the critical angle for channeling at depth $x$ [10] :

$$\psi_c(x) = \left(\frac{2Z_1Z_2e^2}{dE(x)}\right)^{1/2} \left[\frac{1}{2} \ln \left(\frac{Ca}{\rho} + 1\right)\right]^{1/2}$$  \hspace{1cm} (2.22)

$a$ is the Thomas-Fermi screening distance given by $a = 0.8854a_0(Z_1^{2/3} + Z_2^{2/3})^{-1/2}$, where $a_0$ is the Bohr radius. $C$ is a constant ($= 1.732$) [17], $\rho$ is the rms thermal vibration amplitude ($= 0.106\text{Å}$). $E(x)$ is the incident energy at depth $x$, $d$ is the atomic spacing for Si along the [100] axial direction ($= 5.43\text{Å}$) [18].

Studies show that over most of the range of defect densities where the dechanneling is important ($> 0.01$) multiple scattering is the dominant dechanneling mechanism. We have applied the multiple scattering dechanneling formalism developed by Feldman and Rodgers for which:

$$\chi_r(x) = \chi_v(x) + (1 - \chi_v(x)) \exp\left(-\frac{\psi^2(x)}{\Omega^2(x)}\right)$$  \hspace{1cm} (2.23)

where

$$\Omega^2(x) = \frac{\pi}{2} \left(\frac{2Z_1Z_2e^2}{dE(x)}\right)^2 d^2 \ln \left(\frac{1.29aE(x)}{Z_1Z_2e^2} \cdot \frac{M_2}{M_1 + M_2}\right) \int_0^x N_d(x) dx$$  \hspace{1cm} (2.24)

$M_1$ and $M_2$ are the masses and $Z_1$ and $Z_2$ are the atomic numbers of the projectile ($\text{He}^+$) and target atoms (Si) respectively.

Thus, $N_d(x)$ i.e. the number of displaced atoms in the unit volume at depth $x$ may be calculated by an iterative procedure. At the surface, $\Omega^2(0) = 0$ was used to calculate $N_d(0)$, and the defect density at the surface is given by
\[
\frac{N_d(0)}{N} = \frac{[\chi_d(0) - \chi_v(0)]}{[1 - \chi_v(0)]}
\] (2.25)

The quantity \(N_d(x)/N\) is calculated for each subsequent depth interval. The critical angle \(\psi_c\) can be adjusted to make the damage distribution satisfy the criterion that the damage density becomes zero in deep crystalline layers. Using the above formalism, the damage distribution in the lattice, due to MeV Sb ion implantation in Si(100), has been extracted from the RBS/C data. These results have been presented in Chapters 4, 5 and 6.
Bibliography


