7.1 Introduction
This chapter reviews the fundamentals of penetration of energetic ions into solids. It describes the basic physics of how the ions lose energy to the solid, creating damage and the final distribution of these ions after they stop within the solid. In this chapter, we first present a typical theoretical distribution of ion implantation as calculated by the computer programme TRIM (TRansport of Ions in Matter), which is widely used in ion implantation studies. By reviewing this program, and its many description of the physics of ion penetration of matter, we understand the details necessary to understand various phenomena associated with ion penetration and stopping. Results obtained on ion irradiation studies on SBN and BNN ceramics are presented later in the chapter.

7.2 Calculation of implantation range and damage distribution
The calculation of ion implantation distribution can be made using many computer programs. These programs mostly use fitted curves to experimental data, and generate simple distributions for use in very large scale integration (VLSI) calculation. The first unified approach to stopping and range calculation theory was made by Lindhard, Scharff and Schiott and their approach is commonly called the LSS theory [1]. This work brought together the pieces and, bridging approximations were made so that calculations of stopping and range distributions could be made within a single model. The remarkable achievement was the result of over a decade of study by Lindhard and collaborators [1, 2, 3, 4, 5, 6] with the later publications deriving in detail some of the major equations of LSS theory. LSS theory was the peak of stopping and range theory based on statistics of atoms. With this theory it was possible to predict the range of ions in solids—a remarkable achievement considering it was applicable over the entire range of atomic species and energies up to the stopping power maximum [7, 8, 9, 10, 11, 12]. Since it was based on
Thomas-Fermi atoms it was most accurate for atoms with many electrons in the intermediate range when they are neither fully stripped nor almost neutral. The theory naturally shows no shell effects.

The profiles are very accurate or as accurate as the experimental data. However, if we need distributions in materials, which are not included in the experimental database, we can calculate the mean depth of penetration (a mean depth of 0.1 μm may be anywhere from 0.05 to 0.2 μm). This error is due to the use of LSS theory in simulators [1] since it does not allow for any shell structure in the target atoms. Further, if the target is a compound, range prediction is more difficult. Real layer structures often lead to distributions with several peaks, which can not be described by analytic solutions of VLSI simulation programs.

All the above approximations are eliminated if one uses a Monte Carlo calculation, for here the targets can be complex, and even two or three dimensional with the only limitation being the computer memory size which must hold all the interaction details of the target. The Monte Carlo method allows more rigorous treatment of elastic scattering, explicit consideration of surfaces and interfaces and easy determination of energy and angular distributions. In brief, it allows the incorporation of whatever physics we might think is applicable. The prime problem with a Monte Carlo approach is that the calculations take perhaps 1000 times longer than the use of fitted parameter programs. The general practice in VLSI modelling is to use the general purpose simulation programs, based on parameterized experimental distributions, and check any unusual conditions against Monte Carlo calculation of the same event. This section will concentrate on Monte Carlo calculations based on fundamental principles.

The formalism for a Monte Carlo computer programme which simulates slowing down and scattering of energetic ions in amorphous targets has been described in detail by Biersack and Haggmark [13]. This program has been integrated with the extensive 5 volume study of the stopping powers of ions in solids and then written to run on personal computers. The final implementation is called TRIM and is often surtagged with a year to indicate the version number, e.g. TRIM-95. It was developed for determining ion range
and damage distributions as well as angular and energy distributions of back scattered and transmitted ions. The computer program provides particularly high computer efficiency, while still maintaining a high degree of accuracy.

As with other Monte Carlo programs, TRIM follows a large number of individual ion or particle "histories" in a target. Each history begins with a given energy, position, and direction. The particle is assumed to change direction as a result of binary nuclear collisions and move in straight free-flight-paths between collisions. The energy is reduced as a result of nuclear and electronic (inelastic) energy losses, and a history is terminated either when the energy drops below a pre-specified value or when the particle's position is outside the target. The target is considered amorphous with atoms at random locations, and thus the directional properties of the crystal lattice are ignored. This method is applicable to over ten decades of incident ion energies, 0.1 KeV to many GeV depending on the ion mass. The lower limit is due to the inclusion of binary collisions only, while the upper limit results from the neglect of high order relativistic effects. Also, inelastic energy loss due to nuclear reaction is not included.

The nuclear and electronic energy losses or stopping powers are assumed to be independent. Thus, particles lose energy in discrete amounts in nuclear collisions and lose energy continuously from electronic interactions. For low energies, where nuclear scattering and energy loss is particularly important, the program utilises solid-state inter-atomic potentials.

7.3 Distribution parameters: Straggling, Skewness and Kurtosis

These words are names for quantities related to the second, third and fourth moments of the ion distribution. They are important because many VLSI modeling programs require these parameters to create analytic functions of ion implantation distributions. The use of these words in the ion implantation field is different from that in some statistics textbooks. In this field we use mostly the definitions first proposed by B. Winterbon [10]. For convenience we define each moment below in several different standard notations. It is assumed below that the ion trajectory begins perpendicular to the target surface, collinear to the X-axis, and the Y-axis are orthogonal in the target surface plane.
Mean Project Range  
\[ R_p = \frac{\sum x_i}{N} = <x> \]

Lateral Projected Range  
\[ R_y = \frac{\sum |y_i|}{\sqrt{2N}} = <|y|> \]  \( (7-1) \)

Radial Range  
\[ R_r = \frac{\sum (y_i^2 + z_i^2)^{1/2}}{N} \]

Here \( x_i \) is the projected range of ion "i" on the x-axis i.e. the perpendicular distance from the surface to the end of an ion's track; \( \sum x_i = \) sum of the ion ranges; \( \frac{\sum x_i}{N} = \) the mean projected range of \( N \) ions; and \( <x> = \) the mean projected range of all ions. The transverse co-ordinate "y" is treated the same, only the distance is taken in the XY plane.

The mean projected lateral range is zero for a perpendicular beam, so the above lateral range definition averages the absolute values to provide other information on the first moment of the radial, spread. The mean radical range assumes cylindrical symmetry of the ion distribution.

Variance is the second moment of the range distribution, and we show below several identical definitions using various common notations.

\[
\text{Variance} = \frac{\sum (x_i - R_p)^2}{N} = <(x - R_p)^2>,
\]

\[
= \frac{\sum \Delta x_i^2}{N} = <(\Delta x_i)^2>, \quad (7-2)
\]

\[
= <x^2> - <x>^2 = \frac{(\sum x_i^2)}{N} - (R_p)^2.
\]

where  \( \Delta x_i^2 = \) sum of the square of the deviations of the ion ranges from the mean projected range with \( \Delta x_i = (x_i - R_p) \).

Straggling is a word which is used in ion implantation in several ways, and care should be taken to determine the author's definition. Sometimes it is a synonym for variance and sometimes it is defined as the square root of the variance. In other cases an author such as Winterbon, uses normalized definitions such as:
Straggling = \langle \Delta x_i^2 \rangle / \langle x \rangle^2, we use the common definition that straggling is the square root of the variance.

\[
\text{Straggling} = \sigma = \sqrt{\left( \frac{\sum x_i^2}{N} - R_p^2 \right)} = \langle (\Delta x_i)^2 \rangle^{1/2} \\
\text{Radial straggling} = \sigma_r = \sqrt{\frac{\sum (y_i^2 + z_i^2)}{N} - R_r^2} = \langle (\Delta r_i)^2 \rangle^{1/2}.
\]

(7-3)

We define lateral straggling in the same way as range straggling above. (Lateral coordinate are sometimes called Transverse Co-ordinates). For a normally incident beam we can assume cylindrical symmetry for the range distribution; so the mean lateral projected range is zero (i.e. \( R_y = 0 \)). Further, we average the \( Y \) and \( Z \) projected ranges to increase statistical accuracy:

\[
\text{Lateral straggling} = \sigma_l = \sqrt{\frac{\sum ((y_i + z_i) / 2)}{N}}
\]

(7-4)

\[
\text{Skewness} = \gamma = \frac{\langle \Delta x^3 \rangle}{\langle \Delta x^2 \rangle^{3/2}} = \frac{\sum (x_i - R_p)^3}{(N\sigma^3)}
= \frac{\sum (x_i^3 - 3R_p x_i^2 + 3R_p^2 x_i - R_p^3)}{(N\sigma^3)}.
\]

(7.5)

\[
\text{Kurtosis} = \beta = \frac{\langle \Delta x^4 \rangle}{\langle \Delta x^2 \rangle^2} = \frac{\sum (x_i - R_p)^4}{(N\sigma^4)}
= \frac{\sum (x_i^4 - 4R_p x_i^3 + 6R_p^2 x_i^2 - 4R_p^3 x_i + R_p^4)}{(N\sigma^4)}.
\]

(7.6)

In the above definitions, the projected range and the straggling have dimensions of length, while the high moments, skeweness and kurtosis, are dimensionless. Note that we do not include backscattered or transmitted ions in our moment calculations, although in rare occasion this is done. The skewness tells whether the peak is skewed towards the surface (negative values) or away from the surface (positive values). Another way of stating this is that negative skewness indicates that the most probable depth (the peak position) is greater than the mean depth, and positive values indicate the reverse. Kurtosis
indicates the extend of the distribution tails, with a value of 3.0 indicating a Gaussian
distribution. Since both the shallow and deep tails contribute, no simple rule indicates
what a variation from 3.0 means about the ion distribution. In general, values from 0 to 3
indicate abbreviated tails, and values above 3 indicate broad tails.

7.4 Energy loss of SHI in materials

The total stopping cross-section of ions in solids is divided into two parts: the energy
transferred by the ion to the target electrons (called electronic stopping) and to the target
nuclei (called nuclear stopping). The nuclear stopping component is usually considered
separately because the heavy recoiling target nucleus can be assumed to be unconnected
to its lattice during the passage of the ion, and the elastic recoil energy which is
transferred to it can be treated simply as the kinetic scattering of two heavy screened
particles. Separation of the energy loss of the ion into two separate components ignores
the possible correlation between hard nuclear collisions and large inelastic losses to
electronic excitation. It is felt that this correlation probably is not significant when many
collisions are averaged over, as when an ion penetrates a solid, but is of importance for
single scattering studies and for very thin targets [18].

7.5 Universal nuclear stopping powers

The energy transferred during the screened Coulomb collision of two atoms will be
described as a function of two variables, the projectile atom's initial energy, E, and its
impact parameter, p. Here 'p' is defined as the projected offset of the original path of Z_i
from Z_2. Where Z_1 and Z_2 are the charges of the two atoms. If these two variables are
known, then the energy transfer, T, to the target atom is determined simply from
conservation of energy and momentum, as shown in the equation:

$$ T = \frac{4M_1 M_2}{(M_1 + M_2)^2} E_0 \sin^2 \theta \frac{O}{2} = \frac{4E_c M_c}{M_2} \sin^2 \theta \frac{O}{2} $$

(7-5)

where M_1 and M_2 are the masses of atoms, Z_1 and Z_2, and \( \theta \) is the projectile's scattering
angle in center-of-mass coordinates.
The energy lost by the ion per unit path length is defined as \( \frac{dE}{dR} \). This is related to the nuclear stopping cross-section, \( S_n(E) \), by the relation \( dE/dR = N S_n(E) \), where \( N \) = the atomic density of the target. The nuclear stopping power, \( S_n(E) \), is the average energy transferred when summed over all impact parameters; so from equation (7.5) we have:

\[
S_n(E) = \int_{r_{\text{min}}}^{r_{\text{max}}} T(E, \rho) 2\pi \rho \, dp = 2\pi T E^0 \frac{\rho}{2} \int_0^{\theta_{\text{max}}} \sin^2 \frac{\theta}{2} \, p \, dp ,
\]

with the integration's upper limit being the sum of the two atomic radii, \( r_{\text{max}} \), beyond which the inter atomic potential, \( T \), is zero. We use the center of mass transformation unit:

\[
\gamma = 4 M_1 M_2 / (M_1 + M_2)^2 .
\]

For practical calculations, the universal nuclear stopping is

\[
S_n(E_0) = \frac{8.462 \times 10^{-15} Z_1 Z_2 M_1 S_n(E)}{(M_1 + M_2)(Z_1 + Z_2)} eV / (\text{atom/cm}^2)
\]

Where \( \varepsilon \) is a reduced energy introduced by Lindhard [1, 6], with the reduced energy \( \varepsilon \), being calculated as

\[
\varepsilon = \frac{32.53 M_2 E_0}{Z_1 Z_2 (M_1 + M_2)(Z_1 + Z_2)}
\]

and the reduced nuclear stopping being calculated as:

\[
S_n(\varepsilon) = \frac{\ln(1 + 1.1383 \varepsilon)}{2(\varepsilon + 0.01321 e^{21.226} + 0.39593 e^{-2.3})} \quad \text{For } \varepsilon \leq 30 ;
\]

\[
\frac{\ln(\varepsilon)}{2\varepsilon} \quad \text{for } \varepsilon > 30 ;
\]
7.6 Electronic stopping cross-sections

The Lindhard treatment is a many-body self-consistent treatment of an electron gas responding to a perturbation by a charged particle. It naturally includes the polarization of the electrons by the charged particle and the resultant charge screening and the plasma density fluctuations. It treats smoothly both individual electron excitation and collective plasmon excitations without separate 'distant' and 'close' collision processes. Finally, when used with the local-density-approximation it can be directly applied to any target and, for example, the effects of chemical bonding or crystal structure on stopping power are simply evaluated.

Lindhard's approach to the interaction of a particle with a free electron gas makes the following assumptions.

The free electron gas consists of electrons at zero temperature (single electrons are described by plane waves) on a fixed uniform positive background with overall charge neutrality.

The initial electron gas is of constant density.

The interaction of the charged particle is a perturbation on the electron gas.

All particles are non-relativistic.

The electronic stopping of a charged particle in the local density approximation may be stated as:

\[
S_e = \int \rho \left( \frac{\rho}{\rho} \right) Z_1^2 \rho \, dV
\]

(7-12)

where \( S_e \) is the electronic stopping; \( I \) is the stopping interaction function of a particle of unit charge with velocity, \( v \), with a free electron gas of density, \( \rho \); \( Z_1 \) is the charge of the particle, \( \rho \) is the electronic density of the target, and the charged particle integral is performed over each volume element, \( dV \), of the target. (We use this form of a stopping equation because it simply expands to the form needed for heavy ions). The electronic
density of a target atom is normalized so that its atomic number \( Z_2 = \int \rho \, dV \) with the integration over the atomic volume. Each of the three components of Eq. (7-12) are discussed below.

With these assumptions, Lindhard derived the interaction function, \( I \), of Eq. (7-12) as:

\[
I = \frac{4\pi e^4}{mv^2} \frac{i}{\pi \omega_0^2} \int_0^{k' \omega} \omega \, d\omega \left[ \frac{1}{\varepsilon^1(k, \omega)} - 1 \right]
\]

where the longitudinal dielectric constant, \( \varepsilon^1 \), is derived to be:

\[
\varepsilon^1(k, \omega) = 1 + \frac{2m^2 \omega_0^2}{\hbar^2 k^2} \sum_n \frac{f(E_n)}{N} x 
\]

\[
x \frac{1}{\left\{ k^2 + k \cdot k_n - \frac{2m}{\hbar} (\omega - i\delta) \right\}} + \frac{1}{\left\{ k^2 - 2 k \cdot k_n + \frac{2m}{\hbar} (\omega - i\delta) \right\}}
\]

where \( e \) and \( m \) are the charge and mass of an electron; \( \omega \) is the classical plasma frequency defined as: \( \omega_0^2 = 4\pi e^2 \rho / m \); \( E_n \) is the energy and \( k_n \) the wave vector of the electron in the \( n \)th state; \( f(E_n) \) is the distribution function and is an even function of \( k_n \), and \( \delta \) is a small damping factor[18].

7.7 Range of swift heavy ion beams
Knowing that charged particles lose their energy in matter, it is important to know, how far the particles penetrate before they lose all of their energy. If we assume that the energy loss is continuous, the distance penetrated must be a well defined number, ie. The distance is same for all identical particles with the same initial energy in the same type of material. This quantity is called the range of a particle, and depends on the type of material, the particle type and its energy. Most of the phenomena observed during ion bombardement of solids are related to the energy deposition from the incoming ions to the target. In the keV-MeV range the energy deposition is quite high and easily reaches
1000 eV/A^0. For 100 MeV Fe^+ ions in barium sodium niobate ceramics, this is enough to ionize hundreds of monolayers of the specimen.

An important parameter characterizing ion to target energy transfer is the energy loss dE/dX (eV/A^0), defined as the energy deposition per unit length along the ion track. The values of dE/dX changes with ion energy. The maximum value of the energy loss parameter versus depth appears to be near the end of the ion path, where the ion velocity is quite low. The range of projectile ions in a material is determined by the equation

\[ R = \int (dE/dX)^{-1} dE \quad (7-15) \]

When we consider free energy density (eV/mol) as a function of the radius R around the ion path (columnar track) for various ion velocities, a drastic decrease by a 1/R^2 is observed along the radial direction in all cases. For low velocity ions, the energy deposition is confined to a cylinder of a few tens of nanometers in diameters, while in the case of high velocity ions a few hundreds of nanometers can be reached. Processes during track formation may be represented as shown in the figure 7.2 below.

**Figure 7.1** Shows the schematic diagram of processes during track formation.

By electromagnetic interactions, a high concentration of exited and ionized target atoms is produced along the ion path. The released electrons have a broad spectrum of kinetic energies and trigger considerable ionization on their own. The electronic collision cascade (6 electrons) spreads out rapidly and carries away energy and charge from the ion.
trajectory. A core of positive target ions remains. Due to electrostatic repulsion, these ions repel each other, thereby creating vacancies and interstitials (Coulomb explosions), provided that the time for electron-ion recombination is long compared to the coulomb explosion time. The range of this atomic collision cascade defines the core of the latent track and has a diameter of less than 10 nm. The track core is surrounded by a halo region corresponding to the maximum range of the $\delta$-electrons of about 100-1000 nm.

7.8 Irradiation effect of BNN and SBN ceramics with Fe$^+$ ion beam

**Experimental**

Thin discs of thickness 1mm of Barium Sodium Niobate ($\text{Ba}_2\text{Na}_2\text{Nb}_{10}\text{O}_{30}$ and $\text{Ba}_3\text{Na}_4\text{Nb}_{10}\text{O}_{30}$) ceramics, BNN-II modified with Neodymium samples were used for irradiation with 100 MeV Fe$^+$ ions. The discs were irradiated at room temperature, with in the high vacuum chamber maintained at $10^{-7}$ mbar, using the material science beam line at Nuclear Science Center, New Delhi. The fluence was $10^{13}$ ions/cm$^2$ uniformly across the sample. The ion beam current was kept as low as 1 particle nanoampere (1 pnA) to avoid any heating effect. The ion beam was focused to a spot of 1mm$^2$ size and scanned over an area of 10 mm $\times$ 10 mm using a magnetic scanner to irradiate the whole sample uniformly. The fluence was measured by collecting the charge falling on the sample mounted on a ladder placed in a secondary electron-suppressed geometry. The ladder current was integrated with a digital current integrator and the charge pulses were counted. The charge pulses produced were directly proportional to the number of Fe$^+$ ions bombarding on the sample.

Figure 7.2 shows the high vacuum chamber inside which the samples are mounted on a ladder. The connection leads from the ladder to the respective instruments are made, so as to measure the signals produced when the heavy ions are bombarding on the target. The sample to be irradiated is then placed in the path of focused swift heavy ion beam, which is scanning over an area of 10 mm$^2$. After the mounting and necessary connections the high vacuum chamber is then evacuated using a cryopump connected to the chamber. Most of the control of SHI beam is being done from the control room and the control T. V. monitors is used to view the irradiation process. The 100 MeV Fe$^+$ ion
beam current is selected with typical 1 particle nano ampere (1 pnA). When the initial setting are ready, the control valve opened, through which the beam comes to the material beam line. The sample to be irradiated and the ladder in which it mounted is monitored using a CCD camera installed inside the chamber. We can observe the luminescence produced during irradiation with 100 MeV Fe⁺ ions on the samples, which appears as shining spots scanning over the sample. The scanning process mechanism of the Fe⁺ ion beam is similar to the scanning process in a T.V. camera.

**Figure 7.2** The Ultra high vacuum chamber of material science beam line, of the 15 UD pelletron Accelerator, Nuclear Science inside which the samples to be irradiated are mounted.

The following seven compositions of BNN systems were irradiated with 100 MeV Fe⁺ ions.

1. \( \text{BaNa}_2\text{Nb}_{10}\text{O}_{30} \)
2. \( \text{Ba}_3\text{Na}_3\text{Nb}_{10}\text{O}_{30} \)
3. \( \text{Ba}_{2.6}\text{Na}_4\text{Nb}_{10}\text{O}_{30} \)
4. \( \text{Ba}_{2.2}\text{Na}_4\text{Nd}_{0.4}\text{Nb}_{10}\text{O}_{30} \)
5. \( \text{Ba}_2\text{Na}_{4.5}\text{Nd}_{0.5}\text{Nb}_{10}\text{O}_{30} \)
6. \( \text{Ba}_{1.8}\text{Na}_4\text{Nd}_{0.8}\text{Nb}_{10}\text{O}_{30} \)
7. \( \text{Ba}_{1.4}\text{Na}_4\text{Nd}_{0.8}\text{Nb}_{10}\text{O}_{30} \)

The electronic energy loss, nuclear energy loss, projectile range, longitudinal and lateral straggling were calculated and tabulated in Tables.
7. 9 Results and discussion

Electronic energy in the materials can be varied from tens of eV/A° up to a very high value, say 1000 eV/A° by choosing appropriate ions and their energies at the Pelletron Accelerator at NSC. This provides a remarkable flexibility and adequate opportunity to engineer properties of the materials to acquire desired electrical, optical or mechanical properties.

Figure 7.3 shows the nuclear energy loss for various energies of Fe⁺ ion irradiated Ba₃Na₄Nb₁₀O₃₀ ceramics. From the figure it is clear that, the nuclear energy loss is high towards the low energy region. In the KeV range the nuclear energy loss shows a maximum, it reaches 92.72 eV/A° for 70 KeV Fe⁺ ions. The value of nuclear energy loss (dE/dX)_n changes with ion energy. Above 10 MeV the nuclear energy loss slowly decreases over the high energy region up to 1GeV (1000 MeV). At 100 MeV the nuclear energy loss is 1.812 eV/Å.

Figure 7. 4 shows the electronic energy loss for various energies of Fe⁺ ion irradiated on Ba₃Na₄Nb₁₀O₃₀ ceramics. The electronic energy loss (dE/dX)_e increases as ion beam energy increases, reaches a maximum at 65 MeV, then it gradually decreases till 1000 MeV (1 GeV). The maximum electronic energy loss is 1039 eV/Å. At 100 MeV energy for Fe⁺ ion the electronic energy loss calculated is approximately 1003 eV/Å.

From the results obtained from nuclear and electronic energy loss, it is evident that at 100 MeV, the irradiation energy deposition is mainly due to electronic energy loss, where as, nuclear energy loss is negligible. Hence the major energy loss mechanisms undergoing in the Ba₃Na₄Nb₁₀O₃₀ ceramics is induced by electronic energy deposition.

From figure 7. 5 we get a clear picture of ion penetration range in Ba₃Na₄Nb₁₀O₃₀ ceramics, for various ion beam energies. The projected range of Fe⁺ ions continuously increases with ion energy, manifesting a linear relation between Fe⁺ ion energy vs range in the 10 keV-1000 MeV range. The range of 100 MeV Fe⁺ ion in BNN ceramics (calculated using TRIM-95) is 12.67 μm. Since the calculated range of damage is around
Figure 7.3 Shows the nuclear energy loss in Ba$_3$Na$_4$Nb$_{10}$O$_{30}$ ceramics for various energies of Fe$^+$ ion beams (10KeV - 1 GeV).

Figure 7.4 Shows the electronic energy loss in Ba$_3$Na$_4$Nb$_{10}$O$_{30}$ ceramics for various energies of Fe$^+$ ion beams (10KeV - 1 GeV).
Figure 7.5 Shows the TRIM calculation results of Fe$^+$ ion range in Ba$_3$Na$_4$Nb$_{10}$O$_{30}$ ceramic for various energies of Fe$^+$ ion beams (10 KeV - 1 GeV).

Figure 7.6 Shows the calculated results of longitudinal and lateral straggling of Fe$^+$ ion in Ba$_3$Na$_4$Nb$_{10}$O$_{30}$ ceramic for various energies of Fe$^+$ ion beams (10 KeV - 1 GeV).
12 μm, material beyond the damage range will be initially unaffected by the displacement process due to irradiation; however, defect transport into these regions may occur [2]. It is assumed that the ions penetrated in to the target are implanted inside, since the range of 100 MeV Fe$^+$ is less than the thickness of the sample.

Figure 7. 6 shows the variation of longitudinal and lateral straggling of Ba$_3$Na$_4$Nb$_{10}$O$_{30}$ ceramics corresponding to various ion energies. Lateral straggling sharply increases in the low energy regions and then show a saturation region, then increases slowly over the higher energy range, whereas longitudinal straggling increases more rapidly than the former in the higher energy region. The longitudinal and lateral straggling are related to the second moments of the ion distribution in solid materials. They give the parameters to create analytic functions of ion implantation distribution in the target. In the above discussions, the projected range and the straggling have dimension of length. In table 7. 2 we present the values of nuclear, electronic energy loss, projected range, lateral and longitudinal straggling for Ba$_{1.4}$Na$_{1.8}$Nd$_{0.8}$Nb$_{10}$O$_{30}$ ceramic for various values of Fe$^+$ ion beam energy (10 KeV - 1 GeV), calculated using Monte Carlo simulation code-TRIM-95.

Table 7. 1 The values of nuclear, electronic energy loss, projected range, lateral and longitudinal straggling for Ba$_{1.4}$Na$_{1.8}$Nd$_{0.8}$Nb$_{10}$O$_{30}$ ceramic for various values of Fe$^+$ ion beam energy (10 KeV - 1 GeV), calculated using Monte Carlo simulation code - TRIM-95. Stopping Units = eV/A$^6$.

<table>
<thead>
<tr>
<th>Ion Energy (keV)</th>
<th>dE/dx</th>
<th>dE/dx</th>
<th>Projected Range</th>
<th>Longitudinal Straggling</th>
<th>Lateral Straggling</th>
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<td>7.636E+01</td>
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<td>107 A</td>
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<td>172 A</td>
<td>126 A</td>
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<td>9.757E+01</td>
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<td>288 A</td>
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Figure 7.7 shows the nuclear energy loss (eV/A⁰) for 100 MeV Fe⁺ ions of seven samples of barium sodium niobate and BNN substituted with neodymium that have been subjected to irradiation. From the graph when we compare the nuclear energy loss, it gradually increases as Neodymium concentration increases, although the changes are very small (between 1.75 and 1.95 eV/A⁰). The increase in nuclear energy loss can be attributed to the increase in density of the samples as the neodymium content increases.

Similarly, Figure 7.8 shows the electronic energy loss (eV/A⁰) for Fe⁺ ions (100 MeV) of the above cited seven BNN specimens. The electronic energy loss gradually increases as neodymium concentration increases, the changes are noticeable, since the variation is in the range over 967.6-1049 eV/A⁰. The electronic energy loss variation can
Figure 7.7 Shows the nuclear energy loss for different compositions of barium sodium niobate ceramics irradiated with 100 MeV Si\(^+\) ions, calculated using the Monte Carlo simulation code (TRIM-95).

Figure 7.8 Shows the electronic energy loss for different compositions of barium sodium niobate ceramics irradiated with 100 MeV Si\(^+\) ions, calculated using the Monte Carlo simulation code (TRIM-95).
be attributed to increase in density as well as to the compositional changes. Addition of electronic and nuclear energy loss in the BNN ceramic specimen comes with in the range 969.377-1051 eV/Å. Most phenomena observed during ion bombardment of BNN ceramic specimens are related to the energy deposition from the incoming ions to the target. In the 100 MeV range the Fe$^+$ ions penetrate into the target, losing energy constantly to the electron sea. It may penetrate many monolayers before there is a collision with the target atom, which is hard enough to displace that atom and create a vacancy. The energy required for a target atom to leave its site and be pushed far enough away so that it will not immediately pop back into its empty site is called its displacement energy. Typically this energy is about 10 to 25 eV. When such an energetic collision occurs, then the recoiling target atom may have adequate energy to start a collision cascade; where it hits other target atoms, which in turn may recoil into other atoms etc. In BNN ceramics, energy deposition of the range of 969-1051 eV/Å by 100 MeV Fe$^+$ ions is enough to ionize nearly hundred or more monolayers of the sample.

Figure 7. 9 displays the projected range of seven compositions of BNN ceramics. The range of Fe$^+$ ions (100 MeV) is found to decrease as the concentration of neodymium increase. The variations are very small which comes in the range 12-14 µm. The decrease in projected range can be attributed to the increase in density due to the compositional variation of constituent elements in BNN ceramics. From the projected range calculated for Fe$^+$ ions in Barium sodium niobate systems, it is possible that the projectile atoms penetrate more than 1000 unit cells deep inside the surface of the samples creating ion tracks and displacing the target atoms from the track core.

Figure 7. 10 gives the longitudinal and lateral straggling for Fe$^+$ ions in BNN system, both longitudinal and lateral straggling calculated are found to decrease with increase in neodymium concentration. The table 7. 2 presents the calculated values of electronic and nuclear energy loss, projected range, longitudinal straggling and lateral straggling for seven different compositions of barium sodium niobate and modified ceramic systems for 100 MeV Fe$^+$ ion beam.
Figure 7.9  Shows the projected range for seven different compositions of barium sodium niobate ceramics irradiated with 100 MeV Si$^+$ ions, calculated using the Monte Carlo simulation code (TRIM-95).

Figure 7.10  Shows the longitudinal and lateral straggling for seven different compositions of barium sodium niobate ceramics irradiated with 100 MeV Si$^+$ ions calculated using the Monte Carlo simulation code (TRIM-95).
Table 7.1 The calculated values of electronic and nuclear energy loss, projected range, longitudinal straggling and lateral straggling for various compositions of barium sodium niobate and modified ceramic systems.

<table>
<thead>
<tr>
<th>Sample Composition</th>
<th>dE/dx Electronic</th>
<th>dE/dx Nuclear</th>
<th>Projected Range</th>
<th>Longitudinal Straggling</th>
<th>Lateral Straggling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ba_4Na_2Nb_10O_30</td>
<td>9.676E+02</td>
<td>1.777E+00</td>
<td>13.14 μm</td>
<td>6530 Å</td>
<td>8023 Å</td>
</tr>
<tr>
<td>Ba_3Na_4Nb_10O_30</td>
<td>9.886E+02</td>
<td>1.812E+00</td>
<td>12.85 μm</td>
<td>6290 Å</td>
<td>7698 Å</td>
</tr>
<tr>
<td>Ba_2.6Na_1.4Nd_0.2Nb_10O_30</td>
<td>1.003E+03</td>
<td>1.842E+00</td>
<td>12.67 μm</td>
<td>6208 Å</td>
<td>7599 Å</td>
</tr>
<tr>
<td>Ba_2Na_4Nd_0.4Nb_10O_30</td>
<td>1.020E+03</td>
<td>1.878E+00</td>
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<td>6120 Å</td>
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</tr>
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<td>1.026E+03</td>
<td>1.891E+00</td>
<td>12.41 μm</td>
<td>6086 Å</td>
<td>7451 Å</td>
</tr>
<tr>
<td>Ba_8Na_4Nd_0.6Nb_0.4O_30</td>
<td>1.033E+03</td>
<td>1.907E+00</td>
<td>12.32 μm</td>
<td>6046 Å</td>
<td>7401 Å</td>
</tr>
<tr>
<td>Ba_4Na_8Nd_0.8Nb_0.2O_3</td>
<td>1.049E+03</td>
<td>1.942E+00</td>
<td>12.15 μm</td>
<td>5965 Å</td>
<td>7303 Å</td>
</tr>
</tbody>
</table>

An ion penetrates into a target, losing energy constantly to the electron sea, it may go many monolayers before there is a collision with a target atom which is hard to displace atom and create a vacancy. The energy required for a target atom to leave its site and be pushed far enough away so that it will not immediately pop back into its empty site is called its displacement energy. Typically this energy is about 10 to 25 eV. When such an energetic collision occurs, the recoiling target atom may have adequate energy to start a collision cascade, where it hits other target atoms, which in turn may recoil into other atoms, etc. A cascade is usually divided into displacement collisions, vacancy production, replacement collisions and interstitial atoms, as described below.

The number of displacement collisions record how many target atoms are set in motion in the cascade with energies above their displacement energy. A vacancy is the hole left behind when a recoil atom moves from its original site. Replacement collisions reduce the number of vacancies. If a moving atom strikes a stationary target atom and transfers more than its displacement energy to it, and the initial atom, after the collision, does not have enough energy to move onwards, and it is the same element as the atom it struck, then it just replaces that atom in the target and there is no vacancy created, i.e. a replacement collision has occurred. Although this may sound complicated, this
mechanism may reduce the total vacancies by upto 30%. The summation of these types of collisions is

\[ \text{Displacements} = \text{Vacancies} + \text{Replacement collisions} \]

Finally, there are interstitial atoms. When a recoil atom stops and is not a replacement atom, then it becomes an interstitial. These may be summed as:

\[ \text{Vacancies} = \text{Interstitials} + (\text{Atoms which leave the target volume}) \]

If a cascade atom leaves the target volume, it is no longer followed. That is, if it leaves the target front surface or the rear surface, it is discarded. So vacancies occur within the target, and the final resting place of a moving recoil atom can be some distance from its vacancy. If it recoils and leaves the target clearly the sum of interstitials will be less than the number of vacancies by the loss of that atom. Replacement collisions are not part of this equation because each replacement collision reduces the number of vacancies and the number of interstitials by one, leaving the equation in balance.

The calculation of cascades, target displacements, replacement collisions, etc. make certain assumptions which are defined explicitly below:

Assume an incident atom has atomic number \( Z_1 \) and energy \( E \). It has a collision within the target with an atom of atomic number \( Z_2 \). After the collision, the incident ion has energy \( E_1 \) and the struck atom has energy \( E_2 \). Previously specified for the target are energies \( E_d \), the displacement energy, \( E_b \), the binding energy of a lattice atom to its site, and \( E_f \), the final energy of a moving atom, below which it is considered to be stopped.

A displacement occurs if \( E_2 > E_d \) (the hit atom is given enough energy to leave the site). A vacancy occurs if both atoms have enough energy to leave the site (i.e. \( E_1 > E_d \) and \( E_2 > E_d \)). Both atoms then become moving atoms of the cascade. The energy \( E_2 \) of atom \( Z_2 \) is reduced by \( E_b \) before it has another collision. If \( E_2 < E_d \), then the struck atom does not have enough energy and it will vibrate back to its original site releasing \( E_2 \) as phonons.

If \( E_1 < E_d \) and \( E_2 > E_d \) and \( Z_1 = Z_2 \), then the incoming atom will remain at the site and the collision is called a replacement collision with \( E_1 \) released as phonons. The atom in the lattice site remains the same atom by exchange. This type of collision is common
in single element targets with large recoil cascades. If $E_1 < E_d$ and $E_2 > E_d$ and $Z_1 \neq Z_2$, then $Z_1$ becomes a stopped interstitial atom.

Finally, if $E_1 < E_d$ and $E_2 < E_d$, then $Z_1$ becomes an interstitial and $E_1 + E_2$ is released as phonons. If the target has several different elements in it, and each has a different displacement energy, the $E_d$ will change for each atom of the cascade hitting different target atoms.

7. 10 Irradiation of strontium barium niobate with Si$^+$ ions

The following compositions of strontium barium niobate have been irradiated with 100 MeV Si$^+$ ions.

(1) Sr$_{0.75}$Ba$_{0.25}$Nb$_2$O$_6$  (2) Sr$_{0.61}$Ba$_{0.39}$Nb$_2$O$_6$  (3) Sr$_{0.55}$Ba$_{0.45}$Nb$_2$O$_6$  (4) Sr$_{0.50}$Ba$_{0.50}$Nb$_2$O$_6$

(5) Sr$_{0.47}$Ba$_{0.53}$Nb$_2$O$_6$  (6) Sr$_{0.43}$Ba$_{0.57}$Nb$_2$O$_6$  (7) Sr$_{0.43}$Ba$_{0.57}$Nb$_2$O$_6$  (8) Sr$_{0.40}$Ba$_{0.60}$Nb$_2$O$_6$

(9) Sr$_{0.38}$Ba$_{0.62}$Nb$_2$O$_6$.

Thin discs of the above compositions were cut from the SBN ceramic pellets using a crystal cutter. It is then polished on both sides. So as to make both faces parallel. The samples are mounted on the ladder. Point contact with silver paints were made between the irradiated surface and the ladder in order to collect the ladder current produced by SHI Si$^+$ ions with energy 100 MeV. The Si$^+$ ion were accelerated to 100 MeV using the instrumental control mechanism in the main control room. The beam is delivered by opening the main valve. An appropriate beam current of 3 particle nanoampere (pnA) was choosen and it is maintained throughout the irradiation process. ( An increase in particle nanoampere in the beam current means an increase in the incident particle numbers). The fluence or the number of Si$^+$ irradiated is fixed at $1 \times 10^{13}$ particles/cm$^2$ of the sample. The beam is focused to a spot of 1mm, and scanned over the whole sample using the magnetic scanner control circuitry. After the irradiation, the white surface of the discs turned to dark brown. Fluorescence from the specimen are observed during the irradiation process. After completing the irradiation, the samples are kept inside the vaccum, in order to bring the samples to equillibrium condition, because the immediate exposure to atmosphere may induce undesirable chemical reaction and other nuclear phenomena.

Figure 7.11 shows the nuclear energy loss (eV/A$^0$) for various values of Si$^+$ ions on Sr$_{0.75}$Ba$_{0.25}$ Nb$_2$O$_6$. The value of nuclear energy loss (dE/dX)$_n$ changes with
Figure 7.11 Shows the nuclear energy loss in Sr$_{0.75}$Ba$_{0.25}$Nb$_2$O$_6$ for various energies of Si$^+$ ion beams (10KeV - 1 GeV).

Figure 7.12 Shows the electronic energy loss in Sr$_{0.75}$Ba$_{0.25}$Nb$_2$O$_6$ for various energies of Si$^+$ ion beams (10KeV - 1 GeV).
ion energy. From the figure it is clear that the nuclear energy loss is maximum toward the low energy region. At 26 KeV range the nuclear energy loss shows a maximum value of 35.08 eV/Å. It reduces to 0.3093 eV/Å for 100 MeV Fe⁺ ions. Above 100 MeV the nuclear energy loss slowly decreases over the high energy region till 1 GeV.

Figure 7. 12 shows calculations of electronic energy loss for energies of Si⁺ ion irradiated on Sr₀.₇₅Ba₀.₂₅Nb₂O₆ (SBN-75) sample. The electronic energy loss (Sₑ) increases as ion beam energy increases, reaches a maximum at 24 MeV then it gradually decreases till 1 GeV. The maximum electronic energy loss is 494.4 eV/Å. At 100 MeV energy the electronic energy loss calculated is approximately 363.3 eV/Å. Hence from the results obtained from nuclear and electronic energy loss at 100 MeV, it is evident that the irradiation energy deposition is mainly due to electronic energy loss, Sₑ. Here the contribution from nuclear energy loss is small. Hence the major mechanisms undergoing in the SBN-75 ceramics is induced by electronic energy deposition.

Figure 7. 13 shows the TRIM calculation results of ion penetration range in SBN-75 ceramic for various ion beam energies. The projected range of Fe⁺ ions continuously increases with ion energy showing approximately an exponential increase in the 10 KeV-1 GeV range. The range of 100 MeV Si⁺ ions in Sr₀.₇₅Ba₀.₂₅Nb₂O₆ is 25 µm, which is twice that of 100 MeV Fe⁺ ions in BNN. Sample portion beyond penetration range will be initially unaffected by the displacement process; however defect transport into these system may occur.

Figure 7. 14 shows the changes in the longitudinal and lateral straggling of Sr₀.₇₅Ba₀.₂₅Nb₂O₆ corresponding to various ion energies. Lateral straggling gradually increases with ion energy and exhibits a linear relationship. Longitudinal straggling shows more rapid increase with ion energy, when compared to the former. The lateral and longitudinal parameters indicate the second moment of the ion distribution in Sr₀.₇₅Ba₀.₂₅Nb₂O₆. In the above discussion the projected range and straggling have dimensions of length.

In table 7. 3 we present the calculated values of nuclear, electronic energy loss, projected range, lateral and longitudinal straggling for Sr₀.₃₅Ba₀.₂₅Nb₂O₆ ceramic for
Figure 7.13  Shows the calculated results of $\text{Si}^+$ ion range in $\text{Sr}_{0.75}\text{Ba}_{0.25}\text{Nb}_2\text{O}_6$ ceramic for various energies of $\text{Fe}^+$ ion beams (10 keV - 1 GeV).

Figure 7.14  Shows the calculated results of longitudinal and lateral straggling of $\text{Si}^+$ ion in $\text{Sr}_{0.75}\text{Ba}_{0.25}\text{Nb}_2\text{O}_6$ ceramic for various energies of $\text{Fe}^+$ ion beams (10 keV - 1 GeV).
various values of Si\textsuperscript{+} ion beam energy (10 KeV-1 GeV), calculated using Monte Carlo simulation code - TRIM-95.

Table 7.3 The values of nuclear, electronic energy loss, projected range, lateral and longitudinal straggling for Sr\textsubscript{0.35}Ba\textsubscript{0.22}Nb\textsubscript{2}O\textsubscript{5} ceramic for various values of Si\textsuperscript{+} ion beam energy (10 KeV-1 GeV), calculated using Monte Carlo simulation code - TRIM-95. Stopping Units = eV / Å\textsuperscript{0}.

<table>
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<th>Ion Energy</th>
<th>dE/dx Elec.</th>
<th>dE/dx Nuclear</th>
<th>Projected Range</th>
<th>Longitudinal Straggling</th>
<th>Lateral Straggling</th>
</tr>
</thead>
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<td>299 A</td>
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</tr>
<tr>
<td>8.00 MeV</td>
<td>1.441E+02</td>
<td>9.083E-01</td>
<td>8.43 um</td>
<td>1.08 um</td>
<td>1.28 um</td>
</tr>
<tr>
<td>9.00 MeV</td>
<td>1.491E+02</td>
<td>8.291E-01</td>
<td>9.10 um</td>
<td>1.10 um</td>
<td>1.31 um</td>
</tr>
<tr>
<td>10.00 MeV</td>
<td>1.536E+02</td>
<td>7.637E-01</td>
<td>9.75 um</td>
<td>1.11 um</td>
<td>1.33 um</td>
</tr>
<tr>
<td>20.00 MeV</td>
<td>1.787E+02</td>
<td>4.395E-01</td>
<td>15.65 um</td>
<td>1.22 um</td>
<td>1.53 um</td>
</tr>
<tr>
<td>30.00 MeV</td>
<td>1.806E+02</td>
<td>3.155E-01</td>
<td>21.12 um</td>
<td>1.31 um</td>
<td>1.67 um</td>
</tr>
</tbody>
</table>
Figure 7.15 shows the electronic energy loss ($eV/A^0$) for 100 MeV $\text{Si}^+$ ions on nine different compositions of strontium barium niobate ($\text{Sr}_x\text{Ba}_{1-x}\text{Nb}_2\text{O}_6$ with $0.35 \leq x \leq 0.75$). In the chart when we examine the result, the electronic energy loss shows an increasing trend as the strontium concentration increases.

Similarly, figure 7.16 shows the nuclear energy loss, $S_n$ for 100 MeV $\text{Si}^+$ ions for different compositions of the SBN system. The nuclear energy loss shows a very slow increasing trend with strontium content increase. Addition of electronic and nuclear energy loss calculated is within 353-363 $eV/A^0$ range. From the above results it is evident that the energy deposition is mainly due to electronic energy loss. Hence the major mechanisms undergoing in the SBN ceramic system is induced by electronic energy deposition.

Figure 7.17 shows the projected range of all nine SBN compositions. The range of 100 MeV $\text{Si}^+$ is found to decrease as the strontium content ratio increases. The variations are very small which comes in the range 25.5-24.5 $\mu m$. In figure 7.18 we can observe the variations in longitudinal and lateral straggling for 100 MeV $\text{Si}^+$ ions. Both are found to decrease as Sr content increases.
Figure 7.15  Shows the electronic energy loss for different compositions of strontium barium niobate ceramics irradiated with 100 MeV Si+ ions, calculated using the Monte Carlo simulation code (TRIM-95).

Figure 7.16  Shows the nuclear energy loss for different compositions of strontium barium niobate ceramics irradiated with 100 MeV Si+ ions, calculated using the Monte Carlo simulation code (TRIM-95).
Figure 7.17 Shows the projected range for nine different compositions of strontium barium niobate ceramics irradiated with 100 MeV Si$^+$ ions, calculated using the Monte Carlo simulation code (TRIM-95).

Figure 7.18 Shows the longitudinal and lateral straggling for nine different compositions of strontium barium niobate ceramics irradiated with 100 MeV Si$^+$ ions calculated using the Monte Carlo simulation code (TRIM-95).
The electronic energy loss, nuclear energy loss, projected range, longitudinal and lateral straggling were calculated and listed for nine different compositions of strontium barium niobate solid solutions. The results are tabulated in Table 7.4 for 100 MeV Si$^+$ ions.

**Table 7.4** The calculated values of electronic and nuclear energy loss, projected range, longitudinal straggling and lateral straggling for various compositions of Sr$_x$Ba$_{1-x}$Nb$_2$O$_6$ system

<table>
<thead>
<tr>
<th>Sample Composition</th>
<th>dE/dx Electronic</th>
<th>dE/dx Nuclear</th>
<th>Projected Range</th>
<th>Longitudinal Straggling</th>
<th>Lateral Straggling</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sr$<em>{0.73}$Ba$</em>{0.27}$Nb$_2$O$_6$</td>
<td>3.530E+02</td>
<td>2.998E-01</td>
<td>25.40 μm</td>
<td>1.00 μm</td>
<td>9498 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.48}$Ba$</em>{0.52}$Nb$_2$O$_6$</td>
<td>3.514E+02</td>
<td>2.986E-01</td>
<td>25.47 μm</td>
<td>1.00 μm</td>
<td>9406 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.37}$Ba$</em>{0.63}$Nb$_2$O$_6$</td>
<td>3.524E+02</td>
<td>2.994E-01</td>
<td>25.40 μm</td>
<td>9972 Å</td>
<td>9355 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.33}$Ba$</em>{0.67}$Nb$_2$O$_6$</td>
<td>3.530E+02</td>
<td>3.000E-01</td>
<td>25.35 μm</td>
<td>9948 Å</td>
<td>9321 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.47}$Ba$</em>{0.53}$Nb$_2$O$_6$</td>
<td>3.536E+02</td>
<td>3.006E-01</td>
<td>25.31 μm</td>
<td>9924 Å</td>
<td>9286 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.30}$Ba$</em>{0.70}$Nb$_2$O$_6$</td>
<td>3.546E+02</td>
<td>3.014E-01</td>
<td>25.24 μm</td>
<td>9888 Å</td>
<td>9234 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.35}$Ba$</em>{0.65}$Nb$_2$O$_6$</td>
<td>3.562E+02</td>
<td>3.029E-01</td>
<td>25.12 μm</td>
<td>9826 Å</td>
<td>144 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.61}$Ba$</em>{0.39}$Nb$_2$O$_6$</td>
<td>3.579E+02</td>
<td>3.044E-01</td>
<td>25.00 μm</td>
<td>9762 Å</td>
<td>9052 Å</td>
</tr>
<tr>
<td>Sr$<em>{0.75}$Ba$</em>{0.25}$Nb$_2$O$_6$</td>
<td>3.633E+02</td>
<td>3.093E-01</td>
<td>24.61 μm</td>
<td>9562 Å</td>
<td>8764 Å</td>
</tr>
</tbody>
</table>

Knowing that charged particles lose their energy in matter, it is important to know the exact range of the particles in materials. If we assume that the energy loss is continuous the distance penetrated must be a well defined number, i.e., the distance is same for all identical particles with the same initial energy in the same type of material. But experiments done on thin films show that for small thicknesses, all particles manage to pass through. When the thickness is increased to the range of the ions, the ratio of transmitted to incident ion density decreases. The surprising thing is that the ratio does not drop immediately to the background level, as expected of a well defined quantity. Instead the curves slopes down over a certain spread of thickness [17].

The above result is due to the fact that the energy loss is not in fact continuous, but statistical in nature. Indeed two identical particles with the same initial energy will not, in
general, suffer the same number of collisions and have the same energy loss. A measurement with an ensemble of identical particles, therefore, will show a statistical distribution of range centered about some mean value. This phenomenon is known as range straggling. To a first approximation, the distribution is Gaussian in form. The mean value of the distribution is known as mean range and corresponds to the mid point on the descending slope of the above figure. This is the thickness at which roughly half the particles are absorbed. More commonly, however, what is desired is the thickness at which all the particles are absorbed, in that case the point at which the curve drops to the background level should be taken. This point is usually found by taking the tangent to the curve at the midpoint and extrapolating to the zero level. This value is known as the extrapolated or projected range.

From a theoretical point of view, we might be able to calculate the mean range of a particle of a given energy, \( T_0 \), by integrating the \( \frac{dE}{dX} \) formula,

\[
S(T_0) = \int \left( \frac{dE}{dX} \right)^{-1} dE
\]  

(7.16)

This yields the approximate path length traveled. Equation (7.16) ignores the effects of multiple Coulomb scattering which causes the particles to follow a zigzag path through the absorber. Thus the range, defined as the straight-line thickness, will generally be smaller than the total zigzag path length.

As it turns out, however, the effects of multiple scattering are generally small for heavy charged particles, so that the total path length is, in fact, a relatively good approximation to the straight line range. In practice, a semi-emperical formula must be used,

\[
R(T_0) = R_o(T_{min}) + \int \left( \frac{dE}{dX} \right)^{-1} dE
\]  

(7.17)

where \( T_{min} \) is the minimum energy at which the \( \frac{dE}{dX} \) formula is valid and \( R_o(T_{min}) \) is an empirically determined constant which accounts for the remaining low energy behavior of the energy loss. Results accurate to within a few percent can be obtained in this manner. We must emphasize here that the range as calculated by equation (7.17) only
takes into account energy losses due to atomic collisions and is valid only as long as atomic collisions remain the principal means of energy loss. At very high energies, where the range becomes larger than the mean free path for a nuclear interaction or for bremsstrahlung emission, this is no longer true and one must take into account these interactions as well.

*Velocity effect:* In models, which are developed in order to describe the creation of latent tracks, one of the important parameters is the ion velocity. By comparing the energy calculated using TRIM, it appears that the damage is higher at low velocity than at high velocities for the samples. Thus latent track radii are found to increase when irradiation is performed at low velocity and the $dE/dX$ threshold of damage decreases.

By high resolution electron microscope (HREM), Constantani et al. [14] have shown that for low velocity copper irradiation $dE/dX = 134$ KeV/nm (Cu at 0.8 MeV/amu), the latent track is long and cylindrical in contrast to observations at higher velocities [15] for nearly the same velocity of $dE/dX$ and the incident energy of the beam.

Swift heavy ions on their way through matter, lose energy and induce a continuous trail of exited and ionized target atoms. In many solids, the associated secondary processes lead to permanent radiation damage. Due to their highly charged state associated with a high energy transfer, heavy ions are especially suited to create cylindrical zones of irreversible chemical and structural changes. These zones have a diameter of only a few nanometers and are known as latent tracks.

Another phenomenon observed with swift heavy ion irradiation is sputtering. Sputtering is the removal of near-surface atoms from the target. When a surface atom is knocked out by a highly energetic particle or when collision cascades intersect the surface of the specimen, atoms whose energies exceed the surface binding energy get ejected. Surface atoms are less tightly bound than bulk atoms; therefore only the transfer of the sublimation energy is required to eject the atom. When a cascade gives a target atom an energy greater than the "surface binding energy" of that target, the atom may be sputtered. In order to actually get sputtered, the atom's energy normal to the surface must be above the surface binding energy when it crosses the plane of the surface. The
sputtering of a surface is described by a sputtering yield, which is defined as the mean number of sputtered target atoms per incident ion.

The sputtering yield is very sensitive to the surface binding energy. The surface binding energy of an atom to a surface is known for a few materials, but it is common to use the heat of sublimation as an estimate. Typical values are 44.6 eV (N$_2$), 3.55 eV (Cu), 3.91 eV (Pd), 2.97 eV (Ag) and 3.80 eV (Au). For real surfaces, this changes under bombardment due to surface roughness, and also changes due to surface stoichiometry for compounds. Further, sputtering involves mostly the upper monolayer of the target. For targets such as Ni or heavier metals, the electronic energy loss of a target atom moving through the last monolayer is of the order of the surface binding energy; so even monolayer roughness will change the sputtering yield [16].

7.1 References


