COMPUTER SIMULATION OF
ION IMPLANTATION
COMPUTER SIMULATION OF ION IMPLANTATION

by

NABIL GEORGE EL-AGIZI, B.E.Eng., B. Sc.

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AUTHOR:  
Nabil George El-Agizi, B.E.ENG. (Cairo University), B.Sc. (Ain Shams University), Cairo, Egypt

SUPERVISOR:  
Dr. D.A. Thompson

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ABSTRACT

In this work, a computer simulation for ion implantation has been carried out based on a simplified random model. This simulation has been used to obtain range profiles and deposited damaging energy distributions, for any system and for a wide energy range. The obtained distributions show good agreement with the third order Edgeworth expansion approximation of the standard transport theory solution (the WSS theory). By taking into account the motion of the first knock on atoms, as well as the incident ion itself, a good agreement between the simulation and the WSS theory is found for the damage distribution. A random model for dealing with polyatomic targets is presented. Results obtained show good agreement with the available experimental results for range profiles. The simulation includes obtaining a complete picture of the collision cascade (in space and time). The complete picture of the collision cascade is discussed in relation to the recently observed "molecular effect" and explains some available experimental results. The examination of typical cascades suggests that high energy density regions are responsible primarily for the obtained departures from "Linear Cascade Theory".
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CHAPTER 1

INTRODUCTION

Interest in ion implantation as a method to introduce atoms into the surface layer of a solid has been growing steadily for at least a decade. The marked upsurge of interest in ion implantation since mid-sixties can be attributed largely to its potential application as a technique to produce semiconductor devices. Indeed, certain special devices are already being manufactured using this technique.

For successful application of ion implantation it is necessary to resolve the following primary and secondary problems:

Primary problems:
(a) The spatial distribution of the implanted atoms.
(b) The associated radiation damage.

Secondary problems:
(c) The final crystal lattice site of the implanted atoms.
(d) Subsequent removal of the damage by annealing processes.

Determination of the above features of ion implantation are necessary for any solid state device fabrication. This work concentrates on the primary problems (a) and (b). The damage state associated with the implantation processes is studied regardless of the problem of annealing, i.e. at low temperature.

Since in an actual ion implantation process the exact determination
or control of the point at which the ion enters the irradiated crystal is missing, and if we add to this the fact that in an ion implantation process the surface is bombarded by a large number of ions, it becomes clear that the most convenient attack to this problem should be one that deals with statistically averaged quantities. An analytical approach has been carried out by Winterbon, Sigmund and Sanders (1970), by formulating the process in the form of suitable transport equation(s). The solution however, gives average quantities that describe the spatial distribution of implanted atoms and the damage produced during this process, i.e. problems (a) and (b). It should be noted that the complicated behaviour of the moving atoms inside the bombarded solid can not be known analytically. By lattice disorder is meant the atoms displaced from their lattice sites because of collisions with the moving ion and the subsequent motion of these atoms themselves.

An atom is bound to the lattice with a certain energy. Therefore it should receive an amount of energy greater than this binding energy in order that it can leave its site and be set in motion. This minimum amount of energy required to displace an atom, \( E_d \), is called a threshold or displacement energy.

Displaced atoms when they come to rest between the crystalline structure rows form what is called interstitials. The empty lattice site from which the atom is removed is called a vacancy. Both the vacant sites of the displaced atoms and the interstitials are called defects and comprise the radiation damage. Figure 1 shows a schematic representation of this damage which is known as the collision cascade.

The number of vacancies (or interstitials) is expected to be a linear function of the energy available for nuclear collisions, Kinchin
and Pease (1955), Sigmund (1969). This defines the "Linear Cascade Theory" concept.

- Interstitial
- Vacancy
- Incident ion

Incident ion

Fig. 1 A schematic representation of a collision cascade

Departures from linear cascade theory have been recently recorded by the experimental work of Thompson and Walker (1975) and Mitchell et al. (1974), in which the number of displaced atoms has been measured for various ion species and energies by the channeling technique. The results show a non-linear relation between the number of displaced atoms and the energy involved in the disorder production (the energy available for nuclear collisions) in high energy density cases. Energy density is defined as the energy deposited per unit volume of the disordered cascade. In the experiments by Thompson and Walker (1975), the energy density is increased by using molecular ion beams. The cascade volume of a monatomic beam is identical with the cascade volume of a diatomic beam with the same energy
per atom as the monatomic beam (i.e. it has double the monatomic beam energy),
but the nuclear energy deposited into this cascade volume in the molecular
ion case is double that of the monatomic ion. For the very dense damage
cascades resulting from low energy, heavy ion bombardments the number of
displaced atoms, in the case of the molecular beam, is more than double
the number obtained by the monatomic beam. This is known as the "molecular
effect". A suggestion is made that this observed increase in damage is
due to the overlapping of the individual cascades. Figure 2 shows the
measured density, $F_D$ (i.e. the relative number of displaced atoms
within the cascade volume) against the deposited energy, Thompson and
Walker (1975). It can be seen that for $F_D$ less than $10^{-3}$ linear cascade
theory holds, while for greater damage densities a non-linear effect
starts to appear, in the form of a remarkable increase in damage over that
expected by the linear cascade theory.

The number of displaced atoms as measured in the case of mole-
cular irradiation is used to determine an effective displacement energy,$E_d$, using the linear cascade theory. It is found that as the damage
density increases the value of $E_d$ approaches a very low value (below 1eV),
which is of the same order of the heat of melting (or vapourisation) of
the target material (silicon). Figure 3 depicts this fact. The preceeding
suggests the existence of a thermal spike phenomenon, Seitz and Koehler(1956).

This suggestion is still being investigated by many researchers
and currently it is still a hypothesis, although a good analysis supporting
this hypothesis has been given recently by Sigmund (1974).
Fig. 2  Damage Density as a Function of Deposited Energy—
After Thompson (1975)

\[ \bar{E} = \text{Average Damaging Energy per Atom} \]

\[ \bar{E_v} = 50^\circ \text{K} \]

\[ \bar{E_v} = 300^\circ \text{K} \]

\[ \bar{E_v} = 300^\circ \text{K} \text{ after Mitchell (1974)} \]

\[ \bar{E} = \text{Total Incident Energy/Number of Displaced Atoms} \]

Target: Silicon
Fig. 3
Effective Displacement Energy as a Function of Damage Density - Thompson (1975)

Target: Silicon
Irradiation Temperature: 50 K

- Mitchell et al. (1974)
- Thompson and Walker (1975)

Effective Displacement Energy (eV)
It is also suggested that the subcascade structure and not the averaged cascade volume is the relevant parameter in determining the damage density. This subcascade structure cannot be found by the analytical solutions as mentioned before. However, the subcascade structure is attainable by following the motion of the incident ion as it collides with the target atoms till it comes to rest, then following all subsequently moving target atoms in the same way. Figure 1 describes the formation of the cascade. It is clear that this is practically attainable by large high-speed computers. This procedure on a computer is always known as computer simulation of ion implantation. Due to the random models that are sometimes used to simulate the collision cascade, this procedure may be also called a Monte-Carlo technique.

The previously mentioned problems of determining the spatial distribution of the implanted ions and the deposited energy are considered. A computer program is developed to simulate the ion implantation process. The program determines the spatial distribution of the energy deposited by the incident ion along its track. Comparison with available theoretical solutions shows good agreement. A deviation is found between the Monte-Carlo results for range distribution and the experimental results. This deviation is interpreted as an underestimation of the stopping power to the incident ion as given by the analytical solution. This interpretation is consistent with the experimental and Monte-Carlo analysis of Thompson and Robinson (1975). The program also deals with polyatomic targets.

The detailed picture of the collision cascade is obtained by this simulation to be discussed in relation to the previously mentioned molecular effect. Qualitative agreement is found to assist the idea that
high energy density regions form the main parameter in the observed increased damage density over that expected by the linear cascade theory.
CHAPTER 2

CHARACTERISTICS OF ION IMPLANTATION

2.1 General

Ion implantation is the introduction of atoms into the surface layer of a solid substrate by bombardment of the solid with ions, typically in the KeV to MeV energy range. The solid state aspects are particularly broad because of the range of physical properties that are sensitive to the presence of foreign atoms and defects. Use of implantation techniques affords the possibility of introducing a wide range of atomic species and makes it possible to obtain impurity concentrations and distributions of particular interest; in many cases, these distributions would not be otherwise attainable. Recent interest in ion implantation has focussed on the study of dopant behavior in implanted semiconductors and has been stimulated by the possibilities of fabricating novel device structures. This in turn, necessitates the complete understanding of the factors which affect the electrical characteristics of implanted layers; especially in silicon, germanium and some of the III-V semiconductors. These factors are mainly range distributions of dopant species, lattice disorder, and location of dopant species on substitutional and interstitial sites in the lattice.

During almost the last decade most of the theoretical and experimental work was devoted to the task of understanding the energy-loss processes that govern the range distribution, and it is now possible to predict
accurately most of the factors involved. For example, a typical range distribution in an amorphous substrate is approximately Gaussian in shape, and may therefore be characterized by a mean range and a straggling about this mean value. Both these quantities depend on many variables.

Other problems inherent in the use of ion implantation techniques arise from the lattice disorder and radiation damage effects produced by the incident ion. When an implanted ion slows down and comes to rest, it makes a series of violent collisions with lattice atoms. These displaced atoms can in turn displace others, and the net result is the production of highly disordered region around the track of the incident ion (Figure 1).

The overall objective of most ion implantation processes is to produce a region whose electrical characteristics are determined solely by the dopant atoms located at well-defined positions in the semiconductor lattice. It is now possible to determine what type of site an implanted atom will occupy by the channeling-effect measurements.

2.2 Computer Simulation of Ion Implantation

The objective of carrying out a computer simulation of ion implantation is to obtain complete details about the behavior of an energetic ion upon penetration of an amorphous or crystalline target. The computer simulation is used also to trace the recoiling atoms and give a detailed picture of the damage created in a substrate by a bombarding atom. In this section different simulation models will be discussed. Since the understanding of the interaction potentials acting between colliding atoms and the energy range in which every potential model is most accurate is important in radiation damage studies it will be discussed first.
2.2.1 Interaction potentials:

The accuracy of the results that can be obtained by the computer simulation depends on the accuracy by which the potential acting between unlike atoms, or ions and atoms, and between like atoms can be described. For this purpose consider two atoms with masses \( M_1 \) and \( M_2 \), atomic numbers \( Z_1 \) and \( Z_2 \), their nuclei are separated by a distance, \( r \), and between them there is a potential \( V(r) \). This potential involves the many-body interactions of the electrons and the nuclei as well. The first Bohr radius \( a_0 = 0.529 \, \text{Å} \) and \( D \), the interatomic distance (approximately \( 2.5 \, \text{Å} \)), give a reasonable reference points in the scale of separation, \( r \), between the interacting pair of atoms.

The following distance ranges are considered:

(a) When \( a_0 < r < D \) the closed inner shells of the atoms start overlapping, so that some electrons will find themselves in the same region of space occupying similar energy levels. According to the Pauli's Exclusion Principle these electrons should move to higher energy levels (since the lower levels are filled). The energy required for this change in levels is given by the work done to bring the atoms close together, hence constitutes a positive potential energy of interaction. This is a repulsive potential, known as close shell repulsion. For a pair of inert gas atoms (all shells are closed), the potential is approximated as, Mayer (1934), Abrahamson (1963)

\[
V(r) = Ae^{-r/b}
\]  

(2.2.1)

Where \( A \) and \( b \) are constants empirically determined. Equation (2.2.1) is
known as the Born-Mayer potential. It is a good approximation to the interaction potential in the above mentioned region of separations. In radiation damage studies this range of distances between atoms correspond to low energies around the threshold energy \( E_d \), and thus the Born-Mayer potential is appropriate to radiation damage studies at low energies, Sigmund (1969a).

(b) For very small separations, \( r \ll a_o \), the repulsive Coulombic potential between the nuclei dominates and is given by,

\[
V(r) = \frac{Z_1 Z_2 e^2}{r},
\]

where \( e \) is the electron charge.

(c) For distances \( r < a_o \) where there is a possibility that the cloud of electrons enters the nuclear space, the Coulomb potential is reduced, and the resulting potential is referred to as the screened Coulomb potential, Bohr (1948). A fair approximation for describing the effect of the screening electron cloud is,

\[
V(r) = \frac{Z_1 Z_2}{r} e^2 e^{-r/a}
\]

where \( a = \lambda a_o / (Z_1 Z_2)^{1/6} \).

Bohr suggests a value of \( \lambda = 1 \), and to replace \((Z_1 Z_2)^{1/6}\) by \((Z_1^{2/3} + Z_2^{2/3})^{1/2}\).

The screened Coulomb (Bohr) potential equation (2.2.3) is most suitable at high energies where the high energy of an incident ion (or atom) can bring the two particles close together to separations less than \( a_o \).

It is unfortunate that the energy range from the KeV to few MeV, which is of most interest to radiation damage studies is between these two
extreme values where there is no other model for the potential that is accurate as in the case of very low or very high energies.

Brinkman (1962), has suggested a formula that involves the screened Coulomb and the Born-Mayer potentials in an attempt to obtain a potential model that is valid for small and large distances as well. This is given by,

\[ V(r) = Ae^{-r/b} \left(1 - e^{-ar/b}\right) \quad (2.2.4) \]

with \( a = Ab/2Z_1Z_2E_R^2 \)

and \( E_R = 13.6\text{eV} \) is the Rydberg constant, \( A \) and \( b \) as before.

It is mentioned before that the screened Coulomb potential is a good approximation for small distances. An even better approximation, which takes into account the change in electron energy connected with the mutual approach of the nuclei, have been formulated by Firsov (1958). Since the Thomas-Fermi statistical model of the atom is the basis for this formulation the resulting potential is always referred to as the Thomas-Fermi (Firsov) or TF two centre potential. Similar to the screened Coulomb potential, it is written as,

\[ V(r) = \frac{\phi(r)}{r} \quad (2.2.5) \]

where \( \phi(r) \) is known as the screening function. For the Thomas-Fermi potential, the Thomas-Fermi screening function \( \phi_{TF}(r/a) \) for unlike atoms is given by,

\[ \phi_{TF} = \chi([Z_1^{2/3} + Z_2^{2/3}]^{2/3}r/a) \quad (2.2.6) \]
where
\[ a = \lambda a_0 / \left( z_1^{2/3} + z_2^{2/3} \right)^{1/2} \] (2.2.7)
and \( X(\left[ z_1^{2/3} + z_2^{2/3} \right]^{2/3} r/a) \) is a function that is tabulated by Gombas (1949), \( \lambda \) is an adjustable parameter.

The uncertainties which remained over the range of intermediate distances \( \frac{a_0}{2} \leq r \leq a_0 \) prompted Abrahamson (1963), to calculate the potential from first principles. The T.F.D. (Thomas-Fermi-Dirac) statistical model of the atom was employed. This T.F.D. potential is considered to be the most convenient model for the interaction potential. Now different available simulation models are considered.

2.2.2. Simulation models:

The introduction of large high speed digital computers made it possible to describe the behavior of an energetic ion, or atom, inside a solid. Although the effects of ion bombardment on a solid have been extensively studied for the last twenty years, it is still insufficient to get the detailed knowledge on the complicated behavior of the energetic ions in a solid. Lindhard, Scharff and Schiott (1963) (always referred to as the LSS theory), then Winterbon, Sigmund and Sanders (1970) (referred to hereafter as the WSS theory) have developed a comprehensive unified theory of atomic stopping in which nuclear and electronic collisions are treated as independent processes. However, these theories, which are the approximate solution of the transport theory with regard to the
incident ions in a solid, give only accurate quantitative values of average quantities of range and deposited energy distributions. In the meantime, such theories can neither describe nor predict the complicated behavior of the ions inside the solid.

In the early nineteen sixties many authors successfully developed computer simulation models to describe the motion of energetic ions in solids. One of the earliest attempts to simulate the complete cascade resulting from the motion of an incident ion in a random solid was done by Yoshida (1961). A "hard sphere" potential model, Chadderton (1965), commonly used by this time, is used in his simulation. He studied the interstitial-vacancy distribution created by neutron irradiation and came with the conclusion that the damage created is in the form of non-uniform clusters. Other attempts by Beeler (1964a,b) and, Beeler and Besco (1963a, b, 1964) were made to follow the complete cascade, in which the lattice structure was taken into account. In this case, when the lattice structure is taken into consideration, the motion of the ion, or displaced recoils, is no more random. Once the scattering angle of the ion after its first collision is determined (which defines the direction of motion of the ion as a result of a binary collision), the first nearest neighbours are checked to determine the location of the atom for the next collision, then the second nearest neighbours and so on. Simple cubic structures were studied using different interaction potentials including the Born-Mayer and the screened Coulomb, and it was found that the essential features of the cascade are not affected by altering the potential within reasonable
limits.

Another approach was tried at Oak Ridge by Holmes (1964); Robinson & Oen (1963); Holmes, Liebfried, Oen, and Robinson (1962) and Oen, Holmes, and Robinson (1962). By restricting their interest to the movement of only the primary recoil, they were able to make a more detailed calculation for similar expenditure of time. The scattering by lattice atoms was computed exactly for a variety of potentials. The crystal lattice studied was F.C.C. and the potential was chosen to simulate the potential in Cu. Some calculations were also made in random array of atoms. They initiated a recoil atom with a given energy and direction and followed it to rest, where its position was noted. This was repeated many times with a random variety of starting directions to produce a statistically significant distribution of ranges, path lengths or penetrations, suitable for comparison with experiments. This technique of averaging computed solutions with random starting conditions is referred to as the Monte-Carlo method. The above model used by Robinson et al. (1963) is the basis for a more sophisticated program, MARLOWE, which is a good simulation for ion implantation, Robinson and Torrens (1974). The above models, apart from the previous one, consider the slowing down of a moving ion to be mainly due to energy transfer in binary collisions. The energy losses going to ionization and excitation of different atoms surrounding the track of the moving ion, or recoils, are neglected. Ishitani (1972) takes account of both the elastic scattering and the inelastic (electronic) scattering to develop a better model for the range calculations and back scattering of light ions. Robinson and Agamy (1972), then Robinson (1974) considered the variation of the cross-section as the ion moves from one
collision to the next due to the continuous energy loss by ionization and excitation. They also randomized the distance travelled between collisions so that they were able to get better "surface correction" for range and deposited energy distributions. A surface correction problem arises in the analytical models due to the theoretical assumption of an infinite medium, which means that the ion can cross the target surface several times which is clearly not possible.

One useful application of the Monte-Carlo analysis method is to check the validity of the theoretical model (LSS) which has been based upon many simplifying assumptions. Thompson and Robinson (1975) have shown that the electronic stopping cross-section is approximately 60 percent higher than the standard Lindhard value for 10-40 KeV protons in silicon. This resulted from a comparison of the measured damage distributions with those determined by Monte-Carlo calculation technique. Oen and Robinson (1975) in a study of the reflection of light ions from solids have shown that the standard LSS theory overestimates the stopping cross-section at low energies.

So far we have seen that two major advantages arise in the application of the Monte-Carlo analysis technique. Normally, the study of the complicated ion trajectories in a solid, where the analytical solutions fail, and the case with which input parameters can be adjusted to achieve agreement with measured experimental data which acts as a check on the theoretical basis.

The advantages of a random model over the models for crystal
structure approach are:

(a) Collisions with subthreshold energy transfer are ignored in a random model, which reduces computational effort considerably with approximately the same agreement in the obtained results.

(b) In models that take account of the lattice structure simple structures can be, practically, studied.

(c) The random models are relatively easy to program and are simple.
3.1 Introduction

Of fundamental importance in the fabrication of semiconductor devices is control of the spatial distribution of electrically active dopant species. For successful application of the implantation technique to controllably dope semiconductors, it is necessary to understand the mechanisms governing the penetration of implanted atoms such that the spatial distribution of implanted atoms can be predicted.

The theoretical solution to determine the spatial distribution of implanted atoms deals with averages. However, it does not allow for a detailed study of the particular complicated ion trajectories. A convenient method to study these complicated trajectories is by a Monte-Carlo type of analysis.

In this chapter, the transport theory solution as given by Winterbon et al. (1979) is discussed. The essence of this approach rather than the complicated mathematical derivations is the aim of this discussion. It is to be mentioned that this approach, by setting basic integral equations, for determining the range and damage distributions is the same used in obtaining the number of defects, and the partitioning of energy between nuclear and electronic losses. A simplified random simulation model is discussed also.
3.2 The Basic Integral Equations

3.2.1 Binary elastic collisions:

In the energy range of interest to most ion implantation applications, the elastic interaction between a moving particle and another stationary atom, under the effect of a repulsive interaction potential \( V(r) \), is described by classical mechanics.

Figure (4-a) shows the characteristic parameters. \( \theta_1 \) is the scattering angle of the incident ion, \( \theta_2 \) is the scattering angle of the recoil, \( M \) and \( \gamma \) are the mass and velocity, indices 1 and 2 refer to the incident and stationary atom respectively. \( \phi \) is the azimuthal angle, and \( p \) is the impact parameter.

It is most convenient to study this system in the centre of gravity coordinates, by fixing the C.G. and studying the system motion w.r. to this origin. The C.G. is the centre of gravity of \( M_1 \) and \( M_2 \), Figure (4-b). The scattering angle between the scattered ion and the recoiling atom is \( \theta \). The complete analysis of this problem can be found in Goldstein (1957).

The scattering angle \( \theta \), in the C.G. coordinate-system is given by,

\[
\theta = \pi - 2p \int_0^{u_o} \frac{du}{\sqrt{1 - \left[ \frac{V(u)}{E_{rel}} \right] - p^2u^2}} \quad (3.2.1)
\]

where

\[
E_{rel} = \frac{M_2E}{(M_1 + M_2)}
\]

and

\[
u = \frac{1}{r}, \quad u_o = \frac{1}{r_o}
\]
Fig. 4  (a) Binary Collision in Laboratory Coordinate System

(b) Binary Collision in the C.G. Coordinate System
\( r_0 \) = distance of closest approach, and is defined as,

\( V(u_0) \) = asymptotic kinetic energy, and

\( E \) = incident particle energy.

Since the collision is assumed to be elastic, the energy of the recoiling atom can be obtained by keeping the energy and momentum invariants. The recoiling energy, \( T \), is given by

\[
T = T_m \sin^2 \left( \theta / 2 \right),
\]

(3.2.2)

where

\[
T_m = \frac{4M_1 M_2}{(M_1 + M_2)^2} \quad E = \gamma E, \text{ is the maximum energy that can be given to a recoil.}
\]

Thus the outcome of a collision is a scattered particle with energy \( E - T \) and a recoiling atom with an energy \( T \).

It is clear from equation (3.2.2) that for a given energy \( E \), and a specific system of colliding atoms the energy transferred to a recoiling atom is a function of \( \theta \). From equation (3.2.1) and by choosing the appropriate form of the interaction potential, \( V(u) \), it becomes clear that the energy transferred is a function only of the impact parameter, \( p \). The exact solution to the orbital motion of such a system is usually complicated and is not available except for simple interaction potentials, such as the simple Coulomb potential (light ions and high energies) which lead to the well known Rutherford scattering law, Semat (1955).

In most cases, one is interested in the angular distribution of the incident particles. By this it is meant the probability of scattering
of a particle at an angle between $\theta$ and $\theta + d\theta$. All particles having an impact parameter between $p$ and $p + dp$ will be scattered by an angle between $\theta$ and $\theta + d\theta$. The relation governing this correspondence is equation (3.2.1). Due to symmetry (see Figure 3-a), all particles falling on an area $2\pi pdp$ at an impact parameter, $p$, will be scattered by an angle between $\theta$ and $\theta + d\theta$. This introduces the concept of a differential cross-section, $d\sigma$ such that,

$$d\sigma = 2\pi pdp$$  \hspace{1cm} (3.2.3)

Thus a differential cross-section is the probability of an atomic collision with a certain outcome to occur.

From this it is clear that the differential cross-section is not restricted to nuclear collisions, i.e. it can describe the probability of occurrence of any other event. Hence it should be differentiated between a differential cross-section for nuclear collisions, or electronic collisions, or any other type.

As mentioned before, for high energies and light ions, the simple Coulomb interaction potential applies, giving the Rutherford scattering law $d\sigma \propto \sec^4(\theta / 2) dS_R$, where $dS_R$ is an element of a solid angle at $\theta$. Consideration of other more complicated forms of interaction potentials leads to different expressions for the differential cross-section.

One important differential cross-section that is valid, reasonably accurate, over most of the energy ranges of interest to radiation damage studies is that derived by Lindhard et al. (1968). The reason for
the validity of this differential cross-section over a wide range of energies is the fact that the Thomas-Fermi interaction potential is used. An approximation to the Thomas-Fermi differential cross-section for elastic collisions is given by Lindhard (1968) as,

\[ \sigma = \pi a^2 \left( \frac{dt}{2t^{3/2}} \right) f(t^{1/2}) \]  

(3.2.4)

where

- \( a = \) Screening radius = \( \frac{.8853a_o}{Z^{2/3}} \),
- \( a_o = \) First Bohr radius = \( \frac{\hbar^2}{mc^2} = .529A^0 \),
- \( \hbar = 2\pi\hbar \) is Plank's constant, and
- \( m = \) Mass of an electron.

\( Z \) is such that,

\[ Z^{2/3} = Z_1^{2/3} + Z_2^{2/3} \]

\( t = e^2 T/T_m \),

and \( \epsilon = \frac{M_2}{M_1 + M_2} \frac{E \ a}{Z_1 Z_2 e^2} \) is a dimensionless quantity that is usually called the reduced energy.

Again indices 1 and 2 refer to the incident particle and the recoiling atom, respectively.

The function \( f(t^{1/2}) \) is a function that was calculated numerically for collisions of neutral Thomas-Fermi atoms, and is given by

\[ f(t^{1/2}) = \lambda^1 t^{1/6} (1 + (2\lambda^1 t^{2/3})^{2/3})^{3/2} \]  

(3.2.5)

The parameter \( \lambda^1 = 1.309 \) was determined by best fitting. For very low values of \( t \) (low energies) the differential cross-section (3.2.4) corresponds to a potential of the form \( V(r) \propto r^{-1/3} \). For large values of \( t \) (\( t \) greater than 5), equation (3.2.5) reduces to the Rutherford scattering low, i.e.
\[ f(t) = 1/2 \ t^{1/2}. \]

A good piecewise approximation of \( f(t^{1/2}) \), known as a power cross-section approximation is given as,

\[ f(t^{1/2}) = \lambda_m t^{1/2} - \nu \]  

(3.2.6)

This approximation is usually used to give order of magnitude estimates, Sigmund (1974).

For an energetic particle inside a solid, the main energy-loss mechanisms to be considered in radiation damage studies are:

1) The nuclear energy loss, due to transferring energy to the recoils in a series of nuclear collisions. The relations governing this energy transfer has been discussed in the preceding analysis. Now a nuclear stopping power is defined as

\[ S_n = \int \frac{dE}{N \ dR} = \int_{T} T \ d\sigma \]  

(3.2.7)

where

\[ N \] is the number of target atoms per unit volume and \( R \) is a distance. Equation (3.2.7) is the average energy loss by nuclear collisions in travelling a distance \( dR \).

This completes the discussion about the first energy-loss mechanism.

2) The electronic losses:

According to LSS (Lindhard, Scharff and Shiotto (1963)), the electronic stopping power for an incident ion of velocity \( v \leq Zr^{2/3}v_B \), where \( v_B \) is the velocity of the first Bohr orbital electron, is expressed as

\[ S_e = -\frac{d\alpha}{d\rho} = Kn^{1/2} \]  

(3.2.8)
where
\[ K = \xi_e \frac{0.0793 Z_1^{2/3} Z_2^{2/3} (A_1 + A_2)^{3/2}}{(Z_1^{2/3} + Z_2^{2/3})^{3/4} A_1^{3/2} A_2^{1/2}} \]  
(3.2.9)

\[ \xi_e = Z_1^{1/6} \]

\[ \rho = \pi N a^2 \gamma R \quad (\rho \text{ is a dimensionless quantity}), \]

\[ \text{distance travelled, and } A \text{ is the atomic mass number.} \]

Equation (3.2.8) is similar to equation (3.2.7) for electronic stopping power.

At a little higher velocities \( V \geq Z_1^{2/3} V_B \), we should adopt the other relation as

\[ \frac{dE}{dp} = -\left(\frac{dE}{dp}\right)_V = Z_1^{2/3} V_B \]  
(3.2.10)

= constant independent on energy

For much higher velocities \( V \gg Z_1^{2/3} V_B \), the stopping power should be replaced by the Bethe-Bloch formula.

Thus we can write the total stopping powers as,

\[ (-\frac{dE}{dR})_{\text{total}} = (-\frac{dE}{dR})_{\text{electronic}} + (-\frac{dE}{dR})_{\text{nuclear}} \]  
(3.2.11)

The partitioning of energy between electronic and nuclear energy losses has been discussed by Lindhard et al. (1962).

3.2.2 Basic Integral Equations:

To find the basic integral equations, a deposited energy
distribution function \( F(\mathbf{r}, \mathbf{v}) \) is defined such that \( F(\mathbf{r}, \mathbf{v}) \, d^3r \) is
the energy deposited in the volume \( d^3r \).

This gives,
\[
\int F(\mathbf{r}, \mathbf{v}) \, d^3r = E
\]
(3.2.12)

It is a simple matter to find that \( F(\mathbf{r}, \mathbf{v}) \) should satisfy the following transport equation,
\[
\frac{\mathbf{v}}{v} \frac{\partial F(\mathbf{r}, \mathbf{v})}{\partial r} = N \int d\sigma \left[ F(\mathbf{r}, \mathbf{v}) - F(\mathbf{r}, \mathbf{v}^{'}) - F(\mathbf{r}, \mathbf{v}^{''}) \right]
\]
(3.2.13)

where

\( v = |\mathbf{v}| \) is the absolute velocity of the incident particle before
a collision, \( \mathbf{v}' \) its velocity after the collision, and \( \mathbf{v}'' \) is the velocity
of the recoiling atom. \( N \) is the density of target atoms per-unit
volume.

Transport equations similar to (3.2.13) are similarly obtained
for the case of different incident and target atoms, as well as for
polyatomic targets. Sanders (1968) gave the transport equation for the
range of a particle, with atomic number \((Z_1)\), slowing down in a monatomic
target, with atomic number \((Z_2)\) as
\[
\int F(\mathbf{r}, \mathbf{v}) d^3r = 1
\]
(3.2.14a)

\[
\frac{\mathbf{v}}{v} \frac{2}{\sigma} F_R(\mathbf{r}, \mathbf{v}) = N \int d\sigma \left[ F_R(\mathbf{r}, \mathbf{v}) - F_R(\mathbf{r}, \mathbf{v}^{''}) \right]
\]
(3.2.14b)
where \( d\sigma \) is the cross-section for nuclear collisions between the incident ion and the target atoms. In this equation the electronic component of energy loss is ignored.

Now we can see that the main differences between (3.2.13) and (3.2.14) are:

1) For deposited energy we use the cross-section \( d\sigma \), which describes collisions between similar target atoms, while in range calculations we consider only the collisions between the primary and target atoms, since target atom collisions with each other are assumed to have no effect on the motion of the primary and its final position.

2) This consideration in (1) makes the third term in (3.2.13) disappear in (3.2.14) which in turn removes the inhomogeneity in (3.2.13).

The case of a polyatomic target is a generalization of the preceding case. It is a direct matter to see that if \( F_{ij}(\vec{r}, \vec{v})d^3r \) is the average kinetic energy of atoms of type \( j \) as a consequence of the slowing down of a particle of type \( i \), then

\[
\sum_j F_{ij}(\vec{r}, \vec{v})d^3r = E \tag{3.2.15a}
\]

and the corresponding transport equation becomes,

\[
-\frac{\dot{\vec{v}}}{\vec{v}} \frac{\partial}{\partial \vec{r}} F_{ij}(\vec{r}, \vec{v}) = \sum_k N_k \int d\sigma_{(ik)}
\]

\[
[F_{ij}(\vec{r}, \vec{v}) - F_{ij}(\vec{r}, \vec{v}')] - [F_{ij}(\vec{r}, \vec{v}) - F_{ij}(\vec{r}, \vec{v}')] \tag{3.2.15b}
\]
The above equations are not enough to determine \( F_{(ij)}(\vec{r}, \vec{v}) \), and in general are not mathematically tractable. Instead, in most practical problems we need only the distribution of total kinetic energy of all types of target atoms due to the slowing down of a certain ion of type \( i \) say, which are described by a distribution function

\[
F_{(i)}(\vec{r}, \vec{v}) = \sum_j F_{(ij)}(\vec{r}, \vec{v})
\]

which should satisfy

\[
\int F_{(i)}(\vec{r}, \vec{v}) d^3r = E
\]

and

\[
-\frac{\vec{v}}{v} \cdot \frac{\partial}{\partial \vec{r}} F_{(i)}(\vec{r}, \vec{v}) = \sum_k \int d\sigma_{(ik)}
\]

\[
[F_{(ik)}(\vec{r}, \vec{v}) - F_{(i)}(\vec{r}, \vec{v}) - F_{(k)}(\vec{r}, \vec{v})]
\]

A similar equation for range distribution can be directly obtained by replacing \( F_{(i)}(\vec{r}, \vec{v}) \) by \( F_R(\vec{r}, \vec{v}) \) and removing the third term in (3.2.18). Equations (3.2.13), (3.2.15) and (3.2.18) are the basic integral equations for different cases. These equations cannot be solved exactly, but exact average quantities can be found.

The simplified case of a monodirectional source gives a practical distribution for both range and deposited energy. For a plane monodirectional source at \( x = 0 \), perpendicular to the target surface, equations (3.2.12) and (3.2.13) become,

\[
-\int_0^\infty F(x, \vec{v}) dx = E
\]
\[ -\cos \theta \frac{\partial}{\partial x} F(x, \hat{v}) = N \int d\sigma [F(x, \hat{v}) - F(x, \hat{v}')] \]

with

\[ F(x, \hat{v}) = dx \int F(\hat{r}, \hat{v}) dy dz \]

For isotropic flow the deposited energy is a function of \( \eta = \cos \theta \)
(the directional cosine of \( \hat{v} \) w.r. to the \( x \) axis), and the energy \( E \).
Thus by expanding \( F \) in terms of Legendre polynomials,

\[ F(x, \hat{v}) = F(x, E, \eta) = \sum_{\ell=0}^{\infty} [(2\ell + 1) F_{\ell}(x, E)P_{\ell}(\eta)] \]

where

\[ F_{\ell}(x, E) = \frac{1}{2} \int_{-1}^{1} d\eta F(x, E, \eta) P_{\ell}(\eta) \]

The final integro-differential equations for \( F(x, E, \eta) \) can be obtained as,

\[ n \ell F_{\ell-1}(E) + n(\ell + 1) F_{\ell+1}(E) = \]

\[ (2\ell + 1)N \int d\sigma [F_{\ell}^n(E) - P_{\ell}(\cos \phi \gamma)] F_{\ell}(E - T) - P_{\ell}(\cos \phi \gamma)^n F_{\ell}(T)] \]

with

\[ F_{\ell}^0(E) = \delta_{\ell0}E \]

and

\[ F_{\ell}^n(E) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} F_{\ell}(x, E) \quad n = 1, 2, 3 \ldots \]

\[ (3.2.20) \]

\[ (3.2.21) \]

\[ (3.2.22) \]

\[ (3.2.23) \]

\[ (3.2.24) \]
By determining the Legendre expansion coefficients, $F_L(x,E)$, different moments of $F(x,E,\eta)$ can be determined, equation (3.2.24).

It is usually sufficient to find the required distribution using the following assumptions:

1) The depth distribution of ion ranges and deposited energy is close to a Gaussian.

2) The medium is random and infinite.

In this case a weighted Gaussian distribution will be a good approximation.

Baroody (1965), approximated the distribution function of range and deposited energy by expanding the function in terms of Edgeworth series. This gives,

$$F(p,e,\eta) = \frac{f}{\Delta p^{1/2}} \phi_0(\xi) - \frac{\Gamma_1}{6} \phi_3(\xi) +$$

$$\frac{\Gamma_2}{24} \phi_4(\xi) + \frac{\Gamma_3}{120} \phi_5(\xi) + \ldots,$$  \hspace{1cm} (3.2.25)

where $\phi_i$ is the $i$th derivative of a Gaussian distribution.

$\xi = (\bar{p} - \langle p \rangle) / \Delta p^{1/2}$,

$\Gamma_1 = \langle \Delta p^3 \rangle / \langle \Delta p^2 \rangle^{3/2}$,

$\Gamma_2 = \langle \Delta p^4 \rangle / \langle \Delta p^2 \rangle^{2.3}$,

$\gamma$ = 1. for range, and

$\gamma$ = $\nu(e)$ for deposited energy.

$\nu(e)$ is the energy available for nuclear collisions, Lindhard et al. (1963).

The above expansion is used in Chapter 4 to give the theoretical range and damage distributions, for different systems by using Winterbon tables, Winterbon (1975), for the first four moments of the distribution.
3.3 The Proposed Model

Different models have been discussed in Chapter 2, and as can be seen that these are divided into random models, and models that follow the particle in the real space of the lattice taking account for lattice structure. The random models depend on assigning a probability function to a certain quantity, that satisfies a certain physical average. Once the probability of a certain event is known, (the weight of occurrence of this event) a random number is assigned to this probability and the calculations are performed many times to ensure that all probable cases are considered. The proposed model is simple, gives good results as compared with theory and experiment, and is a random model.

Three quantities have to be considered to follow the incident ion (or the whole resulting cascade) collision by collision. These are,

1) The scattering angle, whose probability is determined from the cross-section for nuclear collisions. The probability that an incident projectile will be scattered by an angle \( \theta \), in the C.G. coordinate system, that falls between \( \theta \) and \( \theta + d\theta \) is

\[
p(\theta)d\theta = \frac{d\sigma(\theta, E)}{\pi \int_{\theta_{\text{min}}}^{\theta} \frac{d\sigma}{d\theta} d\theta}
\]  

(3.3.1)

The value of \( \theta_{\text{min}} \) should be taken as zero to account for all possible collisions, but the singularity found in the differential cross-section makes it necessary to assume a minimum of the scattering angle greater than zero. The physical meaning of taking \( \theta_{\text{min}} \) equal to zero is...
considering a collision that transfers zero energy to a recoil, which means that all particles at infinite distances are considered, as well. \( \theta_{\text{min}} \), however, should correspond to a maximum impact parameter of half an interatomic distance. This minimum value of \( \theta \) affects the computation considerably while physically it should have a negligible effect in both range and damage calculations. This has been discussed in detail by Ishitani (1972) in his single collision model.

The above integral can be performed as a function of \( t \), i.e.

\[
p(t)dt = \frac{d\theta(t)}{dt} \int_{t_{\text{min}}}^{t_{\text{max}}} \frac{d\sigma(t)}{dt} dt
\]

(3.3.2)

The value of \( t_{\text{min}} \) is taken to correspond to a transferred energy of \( E_d \). As a check, by a power cross-section approximation, this value corresponds to an impact parameter less than half an interatomic distance.

Now the cumulative distribution function of (3.3.2) is

\[
\int_{t_{\text{min}}}^{t} \frac{d\sigma(t)}{dt} dt / \int_{t_{\text{min}}}^{t_{\text{max}}} \frac{d\sigma(t)}{dt} dt = p_1
\]

(3.3.3)

where \( p_1 \) is a random number between zero and one. It should be noted that \( p_1 \) has to be taken from a uniform distribution. It is also important to notice that for a given value of \( p_1 \), the upper limit "\( t \)" of the integral in (3.3.3) should be found in order to calculate the scattering angle, equation (3.2.2). This means that the integral \( \int_{t_{\text{min}}}^{t} \frac{d\sigma(t)}{dt} dt \), has to be tabulated for different values of \( t \). However, the integral in (3.3.1) is a function of energy, which means that the mentioned tabulation procedure has to be done for different values of incident energy from
maximum transferred energy down to $E_d$ say, Ishitani (1974). However, the integral of (3.3.3) is not a function of energy and one table is sufficient, reducing the computation effort, and computer memory usage.

(2) It is clear that the azimuthal angle, Fig.3, is arbitrary and is taken as

$$\phi = 2\pi p_2$$ (3.3.5)

where $p_2$ is another random number that is between zero and one. It should be pointed out that the choice of $\theta$ (together with $\phi$) insures an isotropic flux density of primaries in a random solid.

(3) The final parameter is the determination of the distance between successive collisions, to complete the simulation of the binary collision cascade. For this purpose, we assume an exponential distribution of the free path, with the average of this distribution as the mean free path $\lambda$ where

$$\lambda = \frac{1}{N_0(E,T)}$$ (3.3.6)

From equation (3.3.6) it is seen that the lattice density is preserved, though the lattice structure is ignored. This resembles the case of a gas, which is particularly correct for amorphous structure and high energies, such that the mean free path is large enough, compared to the interatomic spacing, to justify this assumption.

Let $\ell_i$ be the distance travelled after the $i$th collision, and that,

$$P(\ell_i) d\ell_i = \frac{1}{\lambda_i} e^{-\ell_i/\lambda_i} d\ell_i$$ (3.3.7)
is the probability that a collision occurs at a distance between \( \ell_1 \) and \( \ell_1 + d\ell_1 \) from the \((i - 1)\)th collision. Then the probability that this distance is less than or equal to \( \ell_1 \) is given by,

\[
\int_0^{\ell_1} \frac{1}{\lambda_i(E_i)} e^{-\frac{\ell_1}{\lambda_i(E_i)}} d\ell_1 = \left(1 - e^{-\frac{\ell_1}{\lambda_i(E_i)}}\right)
\]

Equation (3.3.8) is obtained with the assumption that the total cross-section for nuclear collisions does not change (by electronic losses) along the distance between two successive collisions, the assumption which is reasonable for low electronic to nuclear energy loss ratio (heavy ions for example).

The left hand side of (3.3.8) varies from zero to 1, and by assigning a third random number \( \eta \), we have

\[
\eta = 1 - e^{-\frac{\ell_1}{\lambda_i(E_i)}}
\]

Since \((1 - \eta) = p_3\) is another random number between zero and one, we have

\[
\ell_1 = -\lambda_i(E_i) \ln p_3 \quad 0 < p_3 < 1
\]

It can be seen that this is the same expression obtained by Robinson (1974), for the case in which the cross-section for nuclear collisions is constant along the distance travelled between successive collisions. As will be seen in the next chapter, from the results obtained for the analytical, experimental and the Monte-Carlo approaches that the variation of the cross-section for nuclear collisions has no observable effect on
the results obtained. This might have been expected since from equation (3.3.9) the effect of the randomness in choosing the distance travelled between successive collisions is more significant than the change in the mean free path due to the change in the cross-section for nuclear collisions.
CHAPTER 4

A COMPARISON BETWEEN THE ANALYTICAL, EXPERIMENTAL
AND MONTE-CARLO TECHNIQUES FOR RANGE DISTRIBUTIONS

4.1 Introduction

In this chapter, the program developed for the ion implantation simulation is tested by comparing the Monte-Carlo results with those obtained by the analytical solution (the WSS theory) and the experimental data available. For a variety of systems (particle-target pairs) and for different energies, the Monte-Carlo range distributions show good agreement with the Winterbon transport theory solution.

The program is also checked for some other quantities such as the reflection coefficient and the partitioning of energy between electronic and nuclear energy losses. Again a good agreement is found. However, the statistics are not enough to give accurate values for the reflection coefficient.

To achieve good agreement between the measured damage distribution produced by energetic protons and the results obtained by a Monte-Carlo technique, Thompson and Robinson (1975) had to increase the standard Lindhard electronic stopping power by approximately 60%. In this chapter, a similar result is obtained for 30-50 KeV bombarded Boron in Silicon. To fit the Monte-Carlo range distribution to the experimental distribution, obtained by secondary mass spectrometry, Hofker et al. (1975), an increase of
approximately 20% in the standard Lindhard electronic stopping power is necessary.

A random simulation model that deals with binary, or polyatomic targets is also presented. Results obtained show good agreement with the available experimental results.

4.2 Calculations and Results

The model of Chapter 3 is used to obtain the range distributions. A particle with an incident energy $E_0$, and any arbitrary angle to the surface normal, is followed collision by collision starting at the target surface. The incident energy $E_0$ is reduced after each collision by the nuclear energy transferred to a recoil in that collision, equation (3.2.2), and the electronic energy loss by travelling a distance $\ell_i$ between collisions, equation (3.2.8). When the particle energy reaches below a certain cut off energy, $E_f$, the particle is considered to have come to rest. The value of $E_f$ is arbitrary, and should be taken small enough not to affect the value of the range. A typical value might be taken as 25-350 eV.

From equation (3.2.8), by integration, the change in the particle energy due to electronic losses between the $i$th and $(i+1)$th collisions is

$$\Delta E_{ei} = E_i - (\sqrt{E_i} - \frac{k_0 \ell_i}{2})^2,$$

(4.2.1)

where

$$k_0 = \left(\frac{M_1 + M_2}{M_2} \frac{a}{Z_1 Z_2 e^2} \right)^{1/2} / \pi a \sqrt{N_G}^{-1}$$

(4.2.2)
and $K$ is the electronic loss constant defined by equation (3.2.9).

It is possible from equation (3.3.9) that the distance, $L_i$, becomes very large corresponding to a very low value of $p_3$. From equation (4.2.1) it is seen that in such case $\Delta E_{ei}$ will be negative. This result is not physically possible, and requires the constraint of an upper bound on the distance travelled, i.e. the distance travelled from a collision should not exceed the distance that corresponds to the moving particle losing all its kinetic energy, $E_i$, in electronic excitation and ionization. The condition for this is that

$$\Delta E_{ei} \leq E_i, \quad \text{or} \quad L_i \leq 2 E_i^{1/2} K_0 \quad (4.2.3)$$

For the case in which the inequalities (4.2.3) and (4.2.4) are not satisfied, the equalities are taken, and the particle motion is thus terminated.

To reduce the computational effort, the Thomas-Fermi cross-section, equation (3.2.4), is piecewise approximated by a power cross-section. Three different energy ranges are considered:

1) For the dimensionless energy range $10^{-4} \leq \epsilon \leq 10^{-2}$, a power cross-section approximation can be achieved by taking $m = 1/3$, equation (3.2.6).

2) It is known that the 1/3 power cross-section approximation is valid accurately enough in the KeV and upper eV energy range. For the eV energy range a good power cross-section approximation can be achieved by taking $m = 0$, Sigmund (1969a), i.e.

$$f(t^{1/2}) = \lambda_o t^{1/2} \quad , \quad (4.2.6)$$
with

\[ \lambda_0 = 24. \]

This gives a cross-section of the form,

\[ \sigma(t) = \frac{\pi a^2 \lambda_0}{2} (\ln(t) - \ln(t_{\text{min}})) \]  (4.2.7)

3) For other energy ranges, \( \epsilon \geq 10^{-2} \), the cross-section of equation (3.2.4) is used with no approximations. The integral of equation (3.3.3) is then numerically integrated by Gauss quadrature.

It is more accurate, however, to use an energy dependent exponent \( \alpha \), for the power cross-section approximation to achieve smooth fitting.

Fig. 5 Determination of the ion position

Figure 5 depicts the way by which the incident ion is followed. When a particle travels a distance \( l_1 \), after a collision, the components of this distance along the original axes (laboratory axes) \( x_1, y_1 \) and \( z_1 \) are required so that the final spatial position of the ion, or the location
of any collision can be found with respect to these axes.
This can be done by a recurrence relation, Yoshida (1961),
\[
\begin{align*}
\begin{pmatrix}
X_{i+1} \\
Y_{i+1} \\
Z_{i+1}
\end{pmatrix}
&= [B_{i-1}][A_i]
\begin{pmatrix}
0 \\
0 \\
\ell_i
\end{pmatrix}, \\
\end{align*}
\]
where
\[
[B_i] = [B_{i-1}][A_i], \quad i = 1, 2, \ldots, \tag{4.2.9}
\]
\[
[B_0] = I \quad (3 \times 3 \text{ unit matrix, for normal incidence}).
\]
The projection matrix \([A_i]\) is defined as,
\[
[A_i] = \begin{pmatrix}
\cos \phi_i & \cos \theta_i & \sin \phi_i & \sin \theta_i & \sin \phi_i \\
-\sin \phi_i & \cos \theta_i & \cos \phi_i & -\sin \theta_i & \cos \phi_i \\
0 & -\sin \theta_i & \cos \theta_i & 0 & 0
\end{pmatrix} \tag{4.2.10}
\]
\(X_{i+1}, Y_{i+1}, \text{ and } Z_{i+1}\) are the components of \(\ell_i\) along \(x_i, y_i, \text{ and } z_i\). For an incident angle \(\theta_0\) and an azimuthal angle \(\phi_0\), \([B_0] = [A_0]\).

The above equations are applicable for primaries and recoils as well. The scattering angles for the scattered and recoiling atoms are, Goldstein (1957),
\[
\tan \theta_1 = \frac{A_m \sin \theta}{(1 + A_m \cos \theta)}, \tag{4.2.9}
\]
\[
\tan \theta_2 = \frac{\sin \theta}{(1 - \cos \theta)}, \tag{4.2.10}
\]
where \(\theta\) is the scattering angle in the C.G. coordinates, and \(A_m\) is the atomic mass ratio of the target atom to the incident ion.

Program listing with comments is in the appendix.
Table 4.1 shows a quantitative comparison between the Monte-Carlo results and those using the Winterbon transport solution (the WSS theory) as obtained from the tables of Winterbon (1975). For a wide range of atomic mass ratios (~2.5 for light ions down to 0.2 for heavy ions), and for different incident energies, the projected ranges and the range straggling compare well. The Monte-Carlo range and straggling values shown in Table 4.1 are the computed values which are subject to some changes due to statistics. However, good agreement is found.

The partitioning of the deposited energy between nuclear and electronic energy losses as obtained by the Monte-Carlo analysis has been checked. The Monte-Carlo values for the electronic loss percentage, \( \eta_1 \), shown in Table 4.1 is the ratio of the electronic energy loss, by the incident ion only, to the total incident energy. The corresponding tabulated value of the WSS theory, \( \eta \), is the electronic energy lost by the incident ion and all other subsequent recoils, Lindhard (1962).

It is seen from the table that \( \eta_1 \) approaches \( \eta \) for the case of light ions. As the energy deposited by the incident ion through nuclear collisions increases, \( \eta_1 \) becomes much smaller than \( \eta \). The value of \( \eta_1 \) then should be checked by an analytical expression for \( \eta_1 \). This is given by

\[
\eta_1(\epsilon) = \int_{\epsilon_f}^{\epsilon} \frac{S_\epsilon(\epsilon)}{S_\epsilon(\epsilon) + S_\eta(\epsilon)} \, d\epsilon, \tag{4.2.11}
\]

where \( \epsilon_f \) corresponds to some cut off energy \( E_f \). Again for simplicity, a power cross-section approximation is used to find \( \eta_1(\epsilon) \). This gives
<table>
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<tr>
<th>Incident Ion in Si.</th>
<th>Energy (KeV)</th>
<th>Projected Range (A²)</th>
<th>Straggling</th>
<th>Electronic Loss</th>
<th>Reflection Coeff.</th>
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</thead>
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<td>Calculated</td>
<td>WSS</td>
<td>Calculated</td>
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<td>730</td>
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<tr>
<td></td>
<td>100</td>
<td>1075</td>
<td>1251</td>
<td>399</td>
<td>460</td>
</tr>
<tr>
<td>75 As⁺</td>
<td>30</td>
<td>220</td>
<td>225</td>
<td>85</td>
<td>83</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>308</td>
<td>331</td>
<td>117</td>
<td>125</td>
</tr>
<tr>
<td>114 In⁺</td>
<td>30</td>
<td>189</td>
<td>195</td>
<td>63</td>
<td>57</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>445</td>
<td>499</td>
<td>130</td>
<td>154</td>
</tr>
</tbody>
</table>

Table 4.1 - Comparison Between WSS and Monte-Carlo Projected Range, Straggling, Electronic Loss, and Reflection Coefficients
\[ \eta_1(\varepsilon) = \int_{\varepsilon_f}^{\varepsilon} \frac{K_0^{1/2}}{K_0^{1/2} + K_0^{1/3}} \, d\varepsilon \]  

where

\[ K_0 = .981 \]

The above approximation is most suited for the 100 KeV Indium in Silicon case. In this case \( \eta_1(\varepsilon) = 14.8\% \) for \( \varepsilon \) and \( \varepsilon_f \) equal to .21 and \( 7.3 \times 10^{-4} \), respectively. This is consistent with the calculated values. Hence, the partitioning of energy between electronic and nuclear energy losses is found to be in good agreement.

It is important to notice that the average projected range and the straggling might not be a good measure to the distribution unless it is Gaussian or nearly so. Figures 6-11 show the histograms obtained for the normalized range distributions, which show that not only the average projected range or straggling, but also the overall range distribution is in good agreement with the Winterbon calculations.

Figures 6 and 7 give a comparison between the Monte-Carlo results and the WSS theory solution as well as the experimental results of Hofker et al. (1975), for 30 and 50 KeV Boron in Silicon respectively. It is clear from these figures that:

a) The Monte-Carlo and the WSS distributions are in good agreement, nd that

b) they both predict a deeper distribution

If the electronic stopping power is reduced by approximately 20%, the Monte-Carlo histograms fits the experimental most probable depth, and good agreement is obtained between the Monte-Carlo and the experimental distributions.
Fig. 6
Monte-Carlo, WSS and Experimental Normalized Range Distributions for 30 KeV Boron in Silicon
Fig. 7 Monte-Carlo, WSS, and Experimental Normalized Range Distributions for 50 keV Boron in Silicon
Fig. 8

Monte-Carlo and WSS Normalized Range Distributions for 30 KeV Arsenic in Silicon
Fig. 9
Monte-Carlo and Wss Normalized Range Distributions for 50 KeV Arsenic in Silicon
Fig. 10  Monte-Carlo and WSS Normalized Range Distributions for 30 KeV Indium in Silicon
Fig. 11 Monte-Carlo and WSS Normalized Range Distributions For 100 KeV Indium in Silicon
4.3 Binary Targets

Baroody (1969), Sanders (1968) and Schiott (1968) studied different special cases of equation (3.2.18) for the case of range distribution of a particle slowing down in a polyatomic target. It is extremely difficult to solve the transport equation for such problems unless simplifying assumptions are made.

In this work, a random model, that deals with polyatomic targets to give range and damage distributions, is presented.

Beeler and Besco (1962), studied the characteristics of heavy induced radiation damage in binary materials in a two dimensional calculation employing the hard sphere approximation and the Bohr screened potential. As mentioned before, a model that considers the crystal structure is more complicated and considers collisions with the crystal lattice which can be ignored and have no effect on the obtained results. In the case of binary or polyatomic targets, the structure becomes more complicated.

It is clear that the same procedure used before for range and damage calculations can still be used for polyatomic targets. The only additional factor to be considered is the type of collision. A type "i" of collision means a collision with target atoms of type i, i = 1, 2, ..., n; (n ≥ 1).

The following simplifying assumptions are made:

1) The directional properties of the lattice are ignored, i.e. the target is assumed to be amorphous.

2) All cross-sections for nuclear collisions with different types of target atoms have the same energy dependence. Baroody (1969) in his analytical solution of equation (3.2.18) had assumed this assumption also.
A limitation on this assumption arises when the values of the reduced energy \( \varepsilon \) for both types differ considerably for the same incident energy. This might be the case when the target atoms differ considerably in mass.

3) The collision sequence is randomized, since the target is assumed to be amorphous. In a crystal model approach the sequence of collisions will be defined.

4) The occurrence of each type of collision is weighted by the relative cross-section of this type with respect to the sum of the cross-sections of all types.

Let \( p_i(N) \text{d}N \) be the probability that a collision of type \( i \) will occur between collisions number \( N \) and \( N + \text{d}N \) then assumption (4) is

\[
\frac{\int p_i(N) \text{d}N}{\sum_{i=1}^{n} \int p_i(N) \text{d}N} = R_i, \quad i=1, 2, \ldots, n, \quad (4.3.1)
\]

where

\[
R_i = \frac{n_i \sigma_i}{\sum_{i=1}^{n} n_i \sigma_i}, \quad (4.3.2)
\]

\( S \) is the number of collisions, and \( n_i \) is the number of atoms of type "i" in a target molecule.

A good assumption, that has been checked, is that the values of \( R_i \) are constant with energy, which means that the cross-sections of the different target species will keep the same ratio as the incident energy is changed.

If \( Q \) is a random number; \( 0 < Q < 1 \), then a criterion is made to choose the type of collision such that if

\[
q_{ii} < Q < q_{ui} \quad , \quad (4.3.3)
\]
then the collision is of type $i$,

where

$$q_{li} = 1 - \sum_{j=1}^{n} R_j, \quad i=1, 2, \ldots, n \quad (4.3.4)$$

and

$$q_{ui} = q_{li} + R_i, \quad i=1, 2, \ldots, n \quad (4.3.5)$$

The above means that the interval from zero to one has been segmented into values equal to the different values of $R_i$, and if the random number falls between a lower bound $q_{li}$ and an upper bound $q_{ui}$ (the difference between them is $R_i$), then the collision to be considered is of type $i$. In this way the sequence of collisions with different types is randomized and the average relative number of collisions with a certain type, $i$, is equal to $R_i$ (i.e. equal to the area occupied by the cross-sections of this type relative to the area occupied by the cross-sections of all types, as seen on a plane normal to the direction of motion of the ion).

Figure 12 shows the results for the range distribution of 400 KeV Krypton in amorphous Aluminum Oxide, $\text{Al}_2\text{O}_3$. The results of the previously discussed random model for polyatomic targets, are compared to the experimental results of Jespergard et al. (1967), and the Winterbon calculated range distribution for a hypothetical target that has an atomic mass and atomic number equal to the average of the Aluminum and Oxygen atomic mass and atomic number. These averaged values for $\text{Al}_2\text{O}_3$ are 20.2 and 9.96 respectively.

The Monte-Carlo results are seen to be in good agreement with the Winterbon solution (WSS theory) for this type of hypothetical target.
Fig. 12 A Comparison Between Experimental, WSS, and Random Model Range Distributions for 400 KeV Krypton in Amorphous Al₂O₃
(where this is expected to be a good approximation for the case of Al₂O₃). Both the WSS theory solution and the Monte-Carlo distributions predict an average range that is shorter than the experimental average range by approximately 30%. The above deviation found is the same as that mentioned by Jespergard et al. (1967), and a 30% decrease in the analytical average range is found as compared to the measured value.

Before accounting for this difference, certain experimental observations have to be considered. Ormrod et al. (1965); Fastrup et al. (1965), in stopping-power studies for heavy ions in amorphous Carbon have shown that for a given target, the electronic stopping power is not a monotonically increasing function of Z₁, the atomic number of the projectile, as predicted by the LSS theory. Instead, up to 50% oscillations in the electronic stopping power are found around the value predicted by the theory, depending on the value of Z₁. This is called the Z₁ oscillations.

A suggestion was made by Jespergard et al. (1967), that the difference found in Figure 12 is possibly due to an overestimation of the electronic stopping-power as predicted by the theory.

To fit the Monte-Carlo calculated histogram to the measured distribution in Figure 12, the value of K, equation (3.2.8) has to be decreased by approximately 40%. The measured straggling, however, is still much greater than the Monte-Carlo calculated straggling. This was suggested, Jespergard et al. (1967), to be possibly due to certain experimental artifacts (such as nonuniformities in the oxide film thickness of the
target which would tend to increase the observed straggling).

Figures 13 and 14 show a comparison between the Monte-Carlo and the measured range distribution the 80 and 160 KeV cases respectively. It is seen that a good agreement is found. As was also observed by Jespergard et al. (1967), the effect of the $Z_1$ oscillations does not appear for low energies (less than approximately 100 KeV). This is of course expected due to the decrease of the electronic energy-loss component at low energies. The straggling again is greater in the measured distribution, the reason is the same as is mentioned before.
Fig. 13 Experimental and Random Model Range Distributions
For 100 KeV Krypton in Amorphous Aluminum Oxide

80 KeV
Krypton-Al₂O₃
100 Particles
E_f = 50 eV

- Experimental
- Monte-Carlo
Fig. 14
Experimental and Random Model Range Distributions
For 100 KeV Krypton in Amorphous Aluminum Oxide
CHAPTER 5
ENERGY DENSITIES AND MOLECULAR EFFECTS

5.1 Introduction

All standard theoretical treatments of radiation damage assume that the energy per atom within a cascade is sufficiently small to allow dissipation to proceed to whatever level might be appropriate in a given situation. This, in other words, means that uncorrelated binary collisions are assumed to occur in a collision cascade in the form of a Markovian chain (in which the events are assumed to be independent from preceding events), i.e. the collisions with the moving atoms are ignored. If the energy density is increased within a certain volume, as in the case of molecular beam irradiation, this assumption may no longer be valid. Keeping in mind that, by definition, a spike is a limited volume with the majority of atoms temporarily in motion, Seitz and Koehler (1956), one might look at the "molecular effect", discussed in Chapter 1, on the basis of a spike phenomenon. This has been suggested in literature, Sigmund (1974), Mitchell et al. (1974), and Thompson and Walker (1975).

Departures from linear cascade theory, have been experimentally observed as is discussed in Chapter 1. In the case of high energy densities, a nonlinear relation between damage density and deposited energy going to nuclear collisions has been measured, Figure 2. It was also observed that the measured effective displacement energy, $E_d$, approaches the heat of melting (or vaporization) at high energy densities. This suggests
a thermal spike model to be applicable for such energy densities. At the same time, nonlinear effects have been observed at surprisingly low damage densities of \( \sim 10^{-3} \) (which means that a displaced atom exists among a thousand target atoms). This suggests that the particular cascade structure is the more relevant parameter in examining and explaining this nonlinear effect. Actually, a typical cascade structure can more conveniently indicate damage densities, the physical cascade dimensions and the degree of possible overlapping with other cascades initiated at the same entry point (i.e. the case of molecular beam irradiation). This in addition to some other useful information included in a typical cascade structure (such as the ratio of simple defects to amorphous damage regions which can predict possible defect annealing effects), makes it important to try to obtain typical cascade structures.

In this chapter, the model of Chapter 3 is used to generate deposited energy distributions. By considering the motion of the incident particle and primary recoils only, good agreement is obtained with the transport theory solution for the deposited energy distributions. A good agreement also is found in the surface damage, obtained by these two approaches, in the case of heavy ion bombarding. This is apart from the case of light ions Summers et al. (1971). In this way the present calculations provides a good value for the surface damage that is best suited for investigations on sputtering rates.

The complete picture of a collision cascade is obtained and is discussed in relation to the previously discussed nonlinear and molecular effects. The structure of typical cascades initiated by an energetic molecular
light ion show a small chance of overlapping occurring between the individually produced atomic cascades and thus a less pronounced molecular effect. The damage produced by light ions occurs in the form of simple defects along the incident ion trajectory, with one or two dense clusters usually at the end of the ion track. This can explain the nonlinearities in the monatomic irradiation, and the low value of the displacement energy, Figure 3, as the result of these few dense clusters. On the other hand, the particular structure of the individual cascades does not show a significant chance of overlapping and thus predicts that the molecular effect should be negligible. In contrast, cascades for heavy ions are mainly in the form of an entirely amorphous cascade with a prediction of almost 100% overlapping and a very pronounced molecular effect. The almost 100% damage density in a collision cascade obtained by heavy ion irradiation is completely consistent with the formation of an entirely amorphous region. It should be noticed that the examined cascade structures are those of ion species and energies that have been used in obtaining the damage densities in Figure 2, and the results are accordingly discussed. The preceding, in general, is a support of the idea that the high energy density regions are responsible for the previously mentioned nonlinearities and molecular effects that necessitates another model, rather than the branching binary collisions model, to be applicable for high energy densities. This might be a spike model as is pointed out before in literature, Sigmund (1974).

5.2 Deposited Energy Distributions

It is well known that the distribution of ion ranges in a random
medium is determined by an integro-differential equation of the transport type, equation (3.2.14). The same is true for the distribution of deposited energy. As is mentioned in the discussion in section 3.2, there is a difference between the nature of these two types of distributions. While the range distribution concentrates on the end point of the ion trajectory, the deposited energy distribution should consider the motion of all recoils. In general the analytical solution for range profiles and deposited energy distributions, so far as we are concerned assumes the following:

(1) An infinite medium is assumed and the target surface is not accounted for.

(2) The energy binding an atom to the lattice is not considered, i.e. the threshold energy for displacing an atom, \( E_d \), is effectively taken as zero.

(3) The recoiling atoms are assumed to dissipate energy till their energies become zero, i.e. \( E_f \) is taken as zero.

The inclusion of a displacement energy in the calculations, the Monte-Carlo approach, and an effective cut off energy \( E_f \) is an easy job and is not expected to affect the results greatly, apart from the singularity obtained in the angular distribution integration, equation (3.3.5), which is discussed previously.

The first unavoidable assumption of an infinite medium is a questionable assumption, especially if one is concerned with sputtering rates, and backscattering coefficients. The experimental measurements of Summers (1971), show an increase (by a factor of two) in the sputtering rates of Niobium
by protons as compared to the predicted values from transport theory. In Monte-Carlo technique calculations, carried out by Robinson (1974), the calculations show that the transport theory solution underestimates the surface damage, produced by protons on Niobium, by a factor of two, which is consistent with the experimental measurements. In fact, Monte-Carlo calculations implicitly account for the surface correction.

While this is the case for very light ions (light or heavy is always relative to the target), a good agreement between the Monte-Carlo calculations, in the present work, and the transport theory solution for the deposited energy distribution of heavy ions, is found. By considering the motion of the first knocked on atoms (as a first approximation), a good agreement in the overall deposited energy distributions between the Monte-Carlo and the transport solutions is obtained. The assumption that an ion, or a recoil, can cross the target surface back and forth many times (the assumption of an infinite medium) does not seem to be a serious assumption in the case of bombarding with heavy ions. Actually, for heavy ion bombardment, the probability of the incident ion, or a recoil, leaving the target surface due to multiple scattering is very small at low energies. In this way, in assuming that the target atoms, or the incident ion, can cross the target surface back and forth should have no effect on the results. This is supported by the results obtained in the investigation.

Figures 15 and 16 show the calculated deposited energy distributions for 100 KeV Indium and 40 KeV Nitrogen in Silicon, respectively, as compared
Fig. 15  Monte-Carlo and WSS Theory Deposited Energy Distributions for 100 KeV Indium in Silicon
Fig. 16 Monte-Carlo and Transport Theory Deposited Energy Distribution For 40 keV Nitrogen in Silicon
to the transport theory solutions. The histograms give the energy deposited in atomic collision processes by the incident ion along its track. It is clear that as the incident ion becomes lighter the energy it deposits along its track approaches the transport solution of the deposited energy distribution. This becomes a good approximation for very light ions, Robinson (1974). Figure 17 shows the effect of also considering the motion of the primary recoils and their deposited energy into atomic collisions. A good agreement is found.

It is seen that a second correction, by considering the motion of energetic secondary recoils, seems to be unnecessary. However, for more investigation on the validity of the present simulation, all recoils are now considered and complete information on any member of the collision cascade, (energy, position, and time) is now available. The special structure of the cascade and its implications will be considered in the next section. The partitioning of energy into nuclear and electronic energy losses discussed in the preceding chapter is reconsidered.

Table 5.1 shows the values of the electronic energy loss component obtained by considering the motion of all recoils, \( \eta_{\text{tot}} \), as compared to the transport theory solution values, \( \eta \), Winterbon (1975), and the energy lost by the incident ion in exciting and ionizing atoms along its track, \( \eta_1 \). Twenty cascades have been used in each case. The results show good agreement.

The preceding gives one confidence on the validity of the simulation. Now we proceed to studying the special structure of a collision cascade and its implications in the recently observed "molecular effect".
Fig. 17  Monte-Carlo and Transport Theory Deposited Energy Distribution For 30 KeV Indium in Silicon
<table>
<thead>
<tr>
<th>Incident Ion</th>
<th>$^{14}_N^+$</th>
<th>$^{31}_P^+$</th>
<th>$^{75}_As^+$</th>
<th>$^{114}_I$n$^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_0$ keV</td>
<td>40</td>
<td>50</td>
<td>30</td>
<td>50</td>
</tr>
<tr>
<td>$n$ %</td>
<td>57</td>
<td>39</td>
<td>30</td>
<td>32</td>
</tr>
<tr>
<td>$n_1$ %</td>
<td>43</td>
<td>21</td>
<td>9</td>
<td>10</td>
</tr>
<tr>
<td>$n_{tot}$ %</td>
<td>55</td>
<td>37</td>
<td>25</td>
<td>28</td>
</tr>
</tbody>
</table>

Table 5.1 A Comparison on the Partitioning of Energy Between Nuclear and Electronic Energy Losses.
5.3 Spike Phenomena and the Molecular Effect

Before discussing the observed nonlinear and molecular effects, a discussion on spike phenomena seems necessary, since it is anticipated that the reason behind this departure from "Linear Cascade Theory" is the existence of "spike", Sigmund (1974).

In the literature, various types of "spikes" are defined and there is a very great deal of confusion over the terminology in spike theory. Thermal, displacement, plasticity and fission spikes are the most popular forms of spikes. Some authors prefer to put both thermal and displacement spikes into a general class which they call temperature spikes. So far as the molecular effects and the previously mentioned nonlinearities are concerned, thermal and displacement spikes will be considered.

Thermal spikes are usually divided into two types, depending on the nature of the initiating heat source. These are known as spherical and cylindrical thermal spikes. These types are now discussed.

a) When the heat source generating the spike is essentially a point source, a spherical thermal spike occurs. Such heat sources exist during the propagation of a cascade when an atom receives an energy lower than the threshold energy, $E_d$. This quantity of energy should be dissipated by the neighbouring atoms through lattice vibrations. A very useful way to regard this effect is of sudden delivery of heat to a restricted volume of the lattice. However, it should be made clear that equilibrium does not exist within the volume and that the concept of a temperature for the region is not a strictly accurate one. Treatments with this kind of
spike, nevertheless, assume an isotropic, homogeneous, medium and apply the normal, classical, macroscopic laws of heat "conduction", Seitz and Koehler (1956). It should be mentioned that besides the questionable assumption of thermal equilibrium, the small number of the considered atoms in a spike does not allow the thermodynamical approach to apply accurately. Calculations on a typical 300 eV spherical thermal spike shows that a completely molten region surrounds the heat source within a sphere of few tens angstroms radius. This might be the case when we have a cluster of atoms with each atom having energies less than $E_d$.

(b) The thermal spike which has been mentioned above possesses the simplest kind of symmetry, namely that of a sphere. Suppose now that an atom or ion is moving in the crystal and that the energy of the particle is such that the separation between subthreshold collisions is only a few angstroms. The spherical thermal spike due to each vibrating struck atom may now be considered to overlap so that there is a row of excited spheroidal regions. As a first approximation, the energy liberated along this row is assumed to be uniformly distributed, as though there were a line of energy. This spike has cylindrical symmetry and is called a cylindrical thermal spike. The proceeding, (a) and (b) are the commonly used thermal spikes in radiation damage studies.

Another important kind of spikes is the displacement spike. When the energy of a moving ion falls below a value that corresponds to an average distance between collisions that is comparable to the interatomic spacing, a region with the majority of atoms in motion exists. This is known
as a displacement spike. The ion energy that corresponds to a displacement spike depends on the mass of the incident ion and the target atoms.

For any spike, a parameter that can generalize the treatments with all kinds of spike is the energy density. Actually all spikes can be regarded as delivering a certain amount of energy to a given volume in a certain time.

It should be made clear that time factors are possibly very important in determining whether or not spike effects can occur. In other words, it is actually the ratio between the rates at which energy is delivered to, and dissipated from a restricted volume that determines the appearance of the spike effects. It is expected that when the energy is deposited on a much shorter time scale than the time required to dissipate this energy, local heating, even melting or-vapourization, occurs. Sigmund (1974), gave an order of magnitude estimate of a spike lifetime, and comparing this to the cascade lifetime (which is the time required to propagate the cascade) as a function of incident energy, the energy range at which spike effects occur, is obtained. The analysis actually ends up with the following conclusions:

1. At low energies, the cascade lifetime is greater than the spike time constant. Hence no spike effects will occur.

2. At high energies, the energy density in the cascade is insufficient to exceed the sublimation energy. Again no spike effects will occur.

3. At an intermediate energy range, the average energy per atom is high and the lifetime of a spike is greater than the lifetime of a cascade and
thus spike effects occur.

The nonlinearities found in the sputtering yield, Andersen and Bay (1974), occurs in an energy range which coincides approximately with the same energy range predicted by Sigmund calculations. This gives confidence in assuming a spike type of phenomena to be responsible for the nonlinearities of Figure 2. There are, however, two important points related to this discussion; these are:

(I) Sigmund calculations for the average energy per atom is not an accurate measure of the existence of spike effects, since the energy actually appears in the form of localized heat sources. Again this is the questionable assumption of local thermal equilibrium.

(II) Even at high energies, spike phenomena should appear due to the fact that some regions of the cascade will contain high energy density clusters. However, the reason why spike effects are not observed in the sputtering experiments of Anderson and Bay (1974), is that these clusters probably occur deep away from the surface. It is seen that this agreement is best visualized by obtaining the complete picture of the cascade.

Now we proceed showing the experimental and computer simulation evidence for the existence of spikes. Thompson and Nelson (1962), and Andersen and Bay (1974), by experiments on sputtering give evidence on the existence of thermal spikes. Electron microscope observations have indicated the formation of thermal spikes in Silicon bombarded with channelled Indium, Bertolotti et al. (1972). Vineyard (1961) and his co-workers at the Brookhaven National Laboratory have initiated numerical calculations
of radiation damage in crystals. Crystal behaviour is directly simulated by suitably programming a digital computer to solve the simultaneous equations of motion of up to one thousand atoms. Studies on low-energy spikes have been carried out by this simulation. A recoil was started with 100 eV in a model representing copper and the events followed after the cascade was over. The effective temperature was found for each atom by dividing its kinetic energy by $\frac{3}{2} k$ (k is Boltzmann's constant), and isotherms are thus obtained. Quantitative agreement is found between the simulation and the classical heat conduction treatments.

The proceeding is a discussion on the spike phenomena and its implications and an attempt to show that there is evidence on the existence of spikes. Now a further step is taken towards understanding the observed nonlinearities and molecular effects, keeping in mind the proceeding concepts. Two different high-energy density effects should be distinguished:

i. The nonlinear relation between the deposited energy going to nuclear collisions and the number of displaced atoms, Figure 2. It should be noticed that this effect appears in monatomic irradiation.

ii. The "molecular effect", is the observation that the number of defects produced by a molecular ion beam is greater than double the number of defects produced by the equivalent monatomic beam with the same energy per atom.

It has been mentioned before that analytical solutions can only give a measure of the energy density as an averaged quantity. It should be noticed, however, that spikes are in general local effects, such that dealing with averaged quantities may underestimate these effects. This
is a rewording of what was mentioned about the invalidity of a thermal equilibrium assumption (with the atoms having a Maxwell-Boltzmann energy distribution). The prediction of how much enhanced damage due to the spike local heating (or melting) effects over that expected by the simple branching binary collisions model is not an easy task. For example, Sigmund (1974) could predict the energy range at which spike phenomena may be pronounced, which agree with the available experimental measurements. But no model is available to estimate the increased damage due to spikes.

Now typical ion implantation experiments that produced the relation in Fig. 2, will be considered. 20 Kv monatomic Nitrogen in Silicon bombardments produced a damage density $F_D$, of $10^{-3}$ at which nonlinear effects started to appear. The collision cascade of this special case is seen in Figure 18, as obtained by this simulation. The following observations can be made:

I— Considering the encircled cluster "A", the number of interstitials coming to rest in this volume is approximately 15–30, and thus the damage density $F_D$, is approximately 1–10 x, which is 1–2 order of magnitude greater than the averaged damage density of $10^{-3}$. This allows the fact that we have nonlinearities at these energy densities as a consequence of having localized high energy density regions; these damage densities are much greater than would be obtained using the calculated averaged values.

II— Figure 18 shows a typical cascade initiated by a Nitrogen ion on amorphous Silicon. If two ions now enter the target at the same entry point (i.e. the case of molecular ion beam irradiation), it is clear that there is
a very small possibility that the cascades produced by these two ions overlap. Hence the molecular effect should not occur. This is experimentally observed.

It should be pointed out that the displaced atoms of Figure 18 are considered to have come to rest when the energy of any moving atom reaches a value below 35 eV (i.e. $E_p$ is 35 eV), to make the results presentable. A random incident ion has been chosen to represent the common features of the cascade. Although this incident ion travels deep into the substrate, it includes the main features of the cascade. Some other cascades have been observed very close to the surface.

Figure 19 shows the collision cascade for a 20 keV Indium in Silicon. An almost 100% overlap of the cascades of the molecular ion beam can occur. This is again consistent with the experimental results of enhanced "molecular effect". This has been driven out from the examination of more than 20 cascades, with the features of the cascades unchanged. Now it has been shown clearly that the molecular effect is due to primarily the overlapping of different cascades. As a consequence, the energy density is increased. However, the exact determination of the amount of the increased damage due to one type or another, or possibly a combination, of spikes still needs more investigations.
Fig. 19 The Collision Cascade of 20 KeV Indium in Silicon
CHAPTER 6
CONCLUSIONS

This work is a numerical simulation of the ion implantation process, in amorphous targets, based on a simplified random model. A number of points are investigated in this simulation.

(a) Range profiles

(b) Deposited energy distributions

(c) Partitioning of energy between nuclear and electronic energy losses.

(d) Reflection coefficients

(e) Interstitial-Vacancy distributions.

A random model for ion implantation in amorphous polyatomic targets is presented.

Three distinct points have been considered:

1) For a wide energy range and from very heavy to very light ions, good agreement with the analytical transport theory solution is found. Range profiles for 50-50 KeV Boron implanted in Silicon, Hofker et al. (1975), when compared to the present calculations, show that the standard Lindhard electronic power is underestimated by approximately 20%. When the correction is done, (the electronic stopping power is increased by ~20%) the most probable ranges coincide, and good agreement is obtained. The departure of the analytical transport theory solution from the experimental distribution for the case of Boron in Silicon is due to the $E_1$ oscillations.
Deposited energy distributions are obtained and are compared to the transport theory solution. It is found that for heavy ions (atomic mass greater than \(50\)) the contribution of the recoils to the deposited energy distribution is large. It has been found also that the energy deposited by the incident ion and that due to the motion of only the first knock on atoms is enough to give good agreement with the transport theory solution (that accounts for the motion of all recoils), for the deposited energy distributions. A better "surface correction" is obtained by accounting for the motion of only the first knock on atoms and the incident ion.

It is constructive in this simulation to investigate the ratio by which the energy of an incident ion is dissipated between nuclear and electronic energy losses. As a first approximation the total electronic energy losses is taken as the energy lost by the incident particle in exciting and ionizing atoms along its track. This approximation is found to be very crude for heavy ions (atomic mass greater than 50) and is a good approximation for light ions (atomic mass less than 10). For heavy ions, however, this partitioning of energy is found to be in good agreement with the transport theory solution when the electronic energy loss component is taken to be the energy of all moving atoms that goes to excitation and ionization of target atoms, Table 5.1.

The reflection coefficients of the incident particles are calculated and is found in close agreement to the WSS values. Due to insufficient statistics, particularly for small reflection coefficients, the obtained values for the reflection coefficient are not accurate.

2) A random model for amorphous polyatomic targets is presented. The model
is a simple one, yet gives good agreement when compared to the available experimental results. Comparing the obtained range profiles to the experimental data on Krypton in amorphous Al$_2$O$_3$, Jespergård et al. (1967), the effect of the $Z_i$ oscillations is observed. The large straggling obtained by the experiment as compared to the calculated value confirms some features of the experimental technique.

3) The Interstitial-Vacancy distribution is obtained by the present simulation by tracing the motion of all moving atoms. The complete picture of the cascade (in space and time) is used to explain the recently reported departures from "Linear Cascade Theory" and the observed "molecular effects". The following two conclusions are found:

a) A 20 KeV Nitrogen in Silicon, which experimentally gives damage densities greater than the expected values from the "Linear Cascade Theory", has been considered. Although a volume averaged damage density of approximately $10^{-3}$ is estimated, some local damage densities are one to two orders of magnitude greater than the averaged values. This explains the observed nonlinear effect at such low averaged damage densities as a result of local high energy density regions, assisting the suggestions of a spike phenomena to be responsible for these nonlinear effects.

b) Examination of the collision cascades of 20 KeV Nitrogen bombardments in Silicon, it has been found that the cascade structure has a small chance of overlapping with a similar cascade (a random one) initiated at the same point at the surface (the case of a molecular ion beam). This predicts that the molecular effect, in this case, should not appear. Experimentally, in
this case, no molecular effect is observed.

For 20 keV Indium in Silicon, the cascades show an almost 100% overlapping predicting an enhanced molecular effect. Again this is experimentally observed.

The proceeding confirms that the molecular effect is due to cascade overlapping which results in high energy density regions, suggesting a spike model to be more conveniently applied for such high energy densities.

The model of Chapter 3 and its extension in Chapter 4 has been implemented on a CDC-6400 computer which is a 60 bit machine. Care should be taken when using this program on other machines. The program has been carefully programed, and testing the program is done in the form of a comparison between the analytical solution and the calculated results. No further tests have been carried out.
REFERENCES.

A


B

Damage in Solids, Vienna,(43-63).
Proceedings of the International Conference on "Radiation
Damage and Defects in Semiconductors", University of Reading,
U.S.A.,(159-164).
Brinkman, J.A. (1962). Int. Conf. on Crystal Defects in Kyoto,
Japan,(120).

C

Chaderton, L.T. (1965), "Radiation Damage in Crystals", N.Y.,
John Wiley.
F


G


H


I


J


K


M

Mayer, J.B., see under Bleick, W.B.


O


R

Robinson, J.B. (1962). see under Oen, O.S.


S


T

Thompson, D.A. and Walker, R.S. (1975). (To be published).


V


W


Winterbon, K.B. (1975). (To be published).

Y

APPENDIX

PROGRAM LISTING

PROGRAM TST(INPUT,OUTPUT,PUNCH,TAPESINPUT,TAPESOUTPUT,TAPES='PUNC

DIMENSION VA,(3), VA2(3), GAMMA(3), AL(3), C2(3), AK1(3), AK3(3), N

DIMENSION T11000), SIGMA1(1000), X11000), Y11000), Z11000), I11000)

DIMENSION FA1(1000), THETA1(1000), A111000), B111000), C111000), L111000)

DIMENSION VA2(3), VA4(3), CC2(3), OR(3), DP(50), DE(50), DPL(50), N

DIMENSION A1(300), B1(300), C1(300), NG1(200), NUN(200), FD(50), FN(2

DIMENSION SC(2), BCD(1)

COMMON /BCD/ AN
COMMON /BCD/ CM, JN
COMMON /BCD/ HSP
EXTERNAL F11

INPUT PARAMETERS:

1) ATOMIC NUMBER OF THE INCIDENT PARTICLE
2) ATOMIC NUMBER OF THE SECOND CONSTITUENT OF THE BINARY TARGET
3) MASS OF THE INCIDENT PARTICLE
4) MASS OF THE SECOND CONSTITUENT OF THE BINARY TARGET
5) ENERGY OF THE INCIDENT PARTICLE IN EV.
6) EFFECTIVE ENERGY OF A MOVING PARTICLE (EV.)
7) OINS=NUMBER OF TARGET ATOMS PER C2C
8) CO=OUTPUT HISTOGRAM INTERVAL (ANGSTROMS)
9) N=NUMBER OF INCIDENT PARTICLES
11) NO=TAKE TWO VALUES; NO=0 TAKES INTO ACCOUNT THE DISTRIBUTION OF THE ENERGY OF THE FIRST PRIMARY KNOCK-ON RECOILS NO=1 OTHERWISE
12) KH=TAKE TWO VALUES; KH=0 GIVES THE INTERSTITIAL-VACANCY DISTRIBUTION

- 86 -
WH = 0  GIVES THE DISTRIBUTION OF VACANCIES AND THE LOCATION OF ALL ATOMS THAT RECEIVED SUB-THE THRESHOLD ENERGIES (HOT SPOTS)

IBM TAKES TWO VALUES:
IBM = 1  GIVES RANGE PROFILES IN BINARY TARGETS
IBM = 0  OTHERWISE

ADK = A FACTOR THAT IS MULTIPLIED BY THE LINDFARO ELECTRONIC LOSS CONSTANT

KU TAKES TWO VALUES:
KU = 1  GIVES A DISPLAY OF THE INTERSTITIAL-VACANCY DISTRIBUTION ON THE PENTON VEHNER PLOTTER.
KU = 0  OTHERWISE

KUM = NUMBER OF CASCADES TO BE PLOTTED

INPUT DATA:
-------------
FIRST CARD  Z1, Z2, Z3, AM1, AM2  FORMAT(5F6,2)
SECOND CARD  A3, CC, EF, EG, DINS  FORMAT(5F6,2,2E16,8)
THIRD CARD  M, NaN, NOP, MM, IBM  FORMAT(515)
FOURTH CARD  ADK, KU, HM  FORMAT(6,3,213)

READ:
-----
READ (5,121) Z1, Z2, Z3, AM1, AM2
READ (5,122) A3, CC, EF, EG, DINS
READ (5,116) M, NaN, NOP, MM, IBM
READ (5,117) ADK, KU, HM

WRITING INPUT DATA TO BE CHECKED:
------------------------------------
WRITE (6,84)
WRITE (6,101) Z1
WRITE (6,102) AM1
WRITE (6,103) Z2
WRITE (6,104) AM2
WRITE (6,110) EG
WRITE (6,109) MN
WRITE (6,107) M
WRITE (6,106) CC
WRITE (6,114) ADK
WRITE (6,115) KU
IF (IBM .NE. 1) GO TO 1
WRITE (6,110) AM3
WRITE (6,112) Z3
WRITE (6,120) IBM
CONTINUE
**THE ELECTRONIC LOSS COEFFICIENT (K)**

```
DO 4 I=1,2
   P2=2*2
   Q2=AM2
   IF (1.EQ.1) GO TO 2
   P1=2*2
   Q1=AM2
   GO TO 3
2   CONTINUE
   P1=2*2
   Q1=AM1
   CONTINUE
   PP=P1**1.6*0.793*P1***(1./2)*R2***(1./2)*Q1*Q2**(1.5)
   QQ=Q3***(2./3)*P2***(2./3)*Q2**1.5
   VA3(I)=PP/Q3
   CONTINUE
   WRITE (6,105) VA3(I)
   ISTART=0
```

**CALCULATION OF THE DIFFERENT CONSTANTS**

```
AU=2.618**2.5
DE(I)=0.
DO 5 I=1,IM
   DE(I+1)=CO*FLOAT(I)
5   CONTINUE
   DP(I)=0.
   DPL(I)=0.
   NQD(I)=0.
   FD(I)=0.
   CONTINUE
   DO 7 I=1,W
   DO 6 J=1,IM
   FN(I,J)=0.
6   CONTINUE
   CONTINUE
   XA=0.
   YA=0.
```
ZA=0
XA2=0
YA2=0
ZA2=0
AL(1)=AM/AV
GAMMA(1)=4. /AL(1)/(AL(1)**2)
GAMMA(2)=1.
G1=Z**2
G2=Z**2
C(1)=SQR(G1+G2)
C(2)=SQR(1)**2
G3=(/13.6)**2
G4=(C2(1)**2)**2
G5=(C2(2)**2)**2
AK1=0.93**4*AL(1)**4
AK2=0.93**4*AL(1)**2
VA1=C2(1)**2*529**2
VA2=C2(2)**2*529**2
AK3=6545*VA1
AK4=6545*VA2
CC1=AL(1)**2*AL(1)**2*C2(1)/(Z1**2*Z2**13.6)
CC2=C2(1)**2*Z2**2*Z2**3.6
VA3=SQRT(CC1)/(VA1*VA1*VA2)
VA4=SQRT(CC2)/(VA1*VA2)

***********************************************************************
** CALCULATION OF THE DIFFERENT CONSTANTS IN CASE OF **
** BINARY TARGETS. **
***********************************************************************

IF (IBM=EQ.0) GO TO 8
P1=Z1
Q1=AM1
P2=Z2
Q2=AM3
P3=P1((1./6.)*0.7**3**1**.07**3**2.**02**0.7**3)**(1./2.)**Q1**Q2)**(1.5)
Q3=(P1**2.3)**0.7**3**2.**02**0.7**3)**7.5
Q4=0.7**3**1.5**0.7**3**2
VA3=P3/Q3
AL(3)=AM3/AM1
GAMMA(3)=4.*AL(3)/(AL(3)**2)
G3=Z3**2.3**2
C3=SQRT(G1+G2)
G4=(C3(1)**2)**2
AK1=0.93**4*AL(3)**4
VA1=0.93**4*VA(3)
8 CONTINUE
CALL TAB1 (7*SIGMA*N10)
DDE=0
NV=0
NA=0
NOT=0
AVZ=0.
AVX=0.
AVY=0.
AVZ2=0.
RR=0.

IF (IBM#.NE.1) GO TO 9.
VA2(1)=(VA2(1)+VA2(3))/2.
VA2(1)=VA2(1)/ADK.
VA2(3)=VA2(1).
CONTINUE.
VA2(1)=VA2(1)/ADK.
EMIN=.03*GAYA(1)/EG.

******************************************************************************
* CALCULATION OF RANGE PROFILES AND DEPOSITED ENERGY.
* DISTRIBUTIONS.
******************************************************************************

DQ 69 IJ=1:K
JO=0.
KI=0.
NON(IJ)=0.
NOM(IJ)=0.
L1=IJ.
L2=IJ+1.
L3=IJ+2.

IF (IBM#.EQ.1) GO TO 10.
ITYP=1.
CONTINUE.

IQ=0.
IK=1.
J1=1.
NB=1.
EV=EG.
XO=0.
YO=0.
ZO=0.
THQ=0.
PHQ=0.
TIMQ=0.
ICALL=1.

IF (NN#.EQ.1) K1=500.
IF (NN#.EQ.0) K1=1000.
CALL FRANDN (A1,K1,L1).
CALL FRANDN (B1,K1,L2).
CALL FRANDN (C1,K1,L3).
CONTINUE.

D1=A1(J1).
D2=B1(J1).
D3=C1(J1).

******************************************************************************
* CALCULATION OF THE RATIO BETWEEN THE DIFFERENT CROSS-SECTIONS.
* REQUIRED BY THE MODEL FOR POLYATOMIC TARGETS.
******************************************************************************

IF (NSI#.GT.1) GO TO 13.
IF (IBM .NE. 1) GO TO 14
NS1 = 2
DO 12 I = 1, 2
   IF (I .EQ. 1) ITPY = 1
   IF (I .EQ. 2) ITPY = 3
   CALL FOLLOW (TH1, TH2, PH1, PH2, EL, J1, ITPY, T, SIGMA, TK, D1, D2, D3, AL, GA
1          MA, AK1, AK3, VA2, DEC, E, EV, CC, NN, GK, IDL, DLL, DUE, IBM, SIGMAT)
   SO(1) = SIGMAT
   CONTINUE
   SO(1) = 3 * SO(1)
   SO(2) = 2 * SO(2)
   RAT = SQRT(SO(2) / SO(1))
   RATE = RAT
   WRITE (C, 12) RAT
   CONTINUE
   ITPY = 3
   IF (D1 .GT. RAT) ITPY = 1
   CONTINUE
   BB = AK3(I TPY)

THE THREE MAIN PARAMETERS IN THE PARTICLE MOTION ARE DETERMINED
BY CALLING SUBROUTINE FCLLOW.

CALL FOLLOW (TH1, TH2, PH1, PH2, EL, J1, ITPY, T, SIGMA, TK, D1, D2, D3, AL, GA
1          MA, AK1, AK3, VA2, DEC, E, EV, CC, NN, GK, IDL, DLL, DUE, IBM, SIGMAT)

THE DISTANCE TRAVELLED BETWEEN COLLISIONS IS PROJECTED ON THE
LABORATORY AXES AND THE LOCATIONS OF NEW RECOLS ARE STORED BY
CALLING LOCATE.

CALL LOCATE (TH0, PH0, TH1, PH1, TH2, PH2, EL, EV, TK, XO, YO, ZO, J1, ICALL, IQ
2          D1, D2, D3, D1, D2, D3, D1, D2, D3, D1, D2, D3)

IF (NN, EQ. 0. OR. NOP. EQ. 1) GO TO 34
ICALL = 2

REDUCING THE ENERGY BY NUCLEAR ENERGY TRANSFER (TK), AND ELECTRONIC
ENERGY LOSS (DEC).

E = EV - TK - DEC
IF (IQ .EQ. 0) GO TO 15
NOT = NOT + 1
IF (IQ .NE. M) GO TO 69
GO TO 16
CONTINUE
IF (TK .LT. 25.) NON(IJ) = NON(IJ) + 1
NON(IJ) = NON(IJ) + 1
J1 = J1 + 1
IF (EV .GT. GR(HT, ITPY)) GC TO 11
NA = NA + 1
J1 = J1 + 1
A(NA) = X(J1)
B(NA) = Y(J1)
C(NA) = Z(J1)
AVZ = AVZ + Z(J1)
AVX = AVX + X(J1)
AVZ2 = AVZ2 + Z(J1) * Z(J1)
AVX2=AVX2*X(J1)*X(J1)
RR=RR*SORT(J1)*X(J1)*Y(J1)*Z(J1)*Z(J1)
IF (I1=NE,M) GO TO 69
16 CONTINUE
M=1
DOE=DOE/FLOAT(LI)
AVZ=AVZ/FLOAT(LI)
AVZ2=AVZ2/FLOAT(LI)
RR=RR/FLOAT(LI)
RATIO=100*CDE/EG
IF (AVZ2.LT.(AVZ*AVZ)) GO TO 17
STRAGZ=SQRT(AVZ2-AVZ*AVZ)
17 CONTINUE
IF (AVX2.LT.(AVX*AVX)) GO TO 18
STRAGX=(AVX2-(AVX*AVX))**.5
18 CONTINUE
DO 19 I=1,IP
ND(K)=0
19 CONTINUE
NDW=0
DO 21 I=1,NA
DO 22 J=1,IP
IF (C(J).GE.DE(J)+AND.C(I).LT.DE(J+I)) ND(J)=ND(J)+1
IF (ND(J).LT.NDN) GO TO 20
NDN=NDN(J)
NJ=J
20 CONTINUE
21 CONTINUE
22 CONTINUE
IF (NDP.EG.0) GO TO 23
DOE=DOE/FLOAT(M-NCT)
RATIO=100*CDE/EG
WRITE (6,111) RATIO
23 CONTINUE
SUM1=0.
SUM2=0.
DPM=0.
DPLM=0.
DO 25 I=1,IV
DP(I)=DP(I)/FLOAT(M)
IF (DPL(I).LT.DPM) GO TO 24
DPM=DP(I)
24 CONTINUE
SUM1=SUM1+DP(I)
DPLM=UPL(I)/FLOAT(M)
IF (DPLM.LT.DPL) GO TO 25
DPLM=DPL(I)
25 CONTINUE
SUM2=SUM2+DPL(I)
26 CONTINUE
WRITE (6,87)
WRITE (6,88) (DP(I),I=1,IV)
WRITE (6,89) SUM1
WRITE (6,89) SUM2
WRITE (6,89) (DPL(I),I=1,IM)
WRITE (6,91) SUM2
IF (NOP.EQ.1) GO TO 27
WRITE (6,83)
WRITE (6,84) NOT
WRITE (6,85) RR
WRITE (6,86) AVZ
WRITE (6,87) STRAGZ
WRITE (6,88) STRAGZ
WRITE (6,89) RATIO
WRITE (6,90) (NO(J), J=1, IV)
CONTINUE
DPM=DPM+1
DOPLM=DOPLM+1
ITM=ITM+1
DO 28 I=1, ITM
CALL PLOPT (DE(I), DP(I), 4)
CONTINUE
I=ITM+1
GO TO 29
CONTINUE
IF (DP(I).LT.DPM.CM+1.EC.IM) GO TO 30
CALL PLOPT (DE(I), DP(I), 4)
I=I+1
GO TO 29
CONTINUE
CALL OUTPLT
IF (NOP.EQ.1) STOP
ANDN=FLOAT(NUN)*1
NJ=NJ+1
DO 31 I=1, NJ
TNO=FLOAT(NE(I), FLCAT(ADA)
CALL PLOPT (DE(I), TNC, 4)
CONTINUE
I=NJ+1
CONTINUE
IF (TNO.LT.ADN.CR+1.EC.IM) GO TO 33
TNO=FLOAT(NE(I), FLCAT(ADA)
CALL PLOPT (DE(I), TNC, 4)
I=I+1
GO TO 32
CONTINUE
CALL OUTPLT
STOP

*******************************************************************************
** EXACT DAMAGE CALCULATIONS
*******************************************************************************

CONTINUE
IF (IG.EQ.0) GO TO 35
NOT=NOT+1
IF (IG.EQ.1) GO TO 36
GO TO 69
CONTINUE
IF (IK.LT.GR(ITYP)) GC GO TO 36
NV=NV+1
CONTINUE
ICALL=2
37 CONTINUE
IF (JKGE.0F(IYP)) ICOD(JJ)=10
JK=JK-1
IF (EV.GT.GR(IYP)) GO TO 10
IF (EV.LT.GR(IYP)) GO TO 39
ZF=Z(JJ)
38 KIM=ICM
DO 38 KIM=1,LM
IF (ZF.LT.DE(KIM).OR.ZF.GE.DE(KIM+1)) GO TO 38
DP(KIM)=OP(KIM)+EV
CONTINUE
39 IF (JM.EQ.1) GO TO 40
JM=JM+1
40 CONTINUE
IF (MM.EQ.0) GO TO 41
ICOD(JJ)=9
IF (IYP.EQ.2) GO TO 41
ICOD(JJ)=2
41 CONTINUE
NB=NB+1
42 NT=J-JK
CONTINUE

CRITERION FOR TERMINATING THE CASCADE AND SETTING INITIAL
VALUES FOR THE NEW RECOILS TO BE FOLLOWED.

43 IF (N0P.EQ.1) GO TO 44
44 IF (IK.GT.(J-1)) GO TO 49
45 IF (ICOD(IK).EQ.10) GO TO 47
46 CONTINUE
GO TO 43
47 IF (N0P.EQ.0) GO TO 46
48 IF (E1(K).GT.JR) GO TO 49
49 IF (E1(K).GT.EMIN) GO TO 47
IK=IK+1
GO TO 45
46 CONTINUE
CONTINUE
IF (IK.LE.1040) GO TO 48
WRITE (5,113)
CALL EXIT
CONTINUE
EV=V(K)
X0=X(K)
Y0=Y(K)
Z0=Z(K)
TH0=THET(K)
PH0=PHAT(K)
IK=IK+1
48 IYP=2
II=0
ICALL=1
GO TO 11
CONTINUE

CALCULATIONS AND OUTPUT RESULTS

IF (IS=E EQ .0) GO TO 50
IF (IJ=EQ .M) GO TO 22
CONTINUE

PLOTTING THE INTERSTITIAL-VACANCY DISTRIBUTION ON THE BESON LEHMEN PLOTTER

IF (KJ=NE .1 OR IJ=NE .1) GC TO 60
CALL LETTER (5,5,90,5,2,5,SHNABIL)
CALL PLOT (4,0,0,3)
CALL PLOT (2,1,3)
CALL PLOT (2,1,2,1)
CALL PLOT (14,1,2)
CALL PLOT (2,1,2)
CALL LETTER (36,15,90,1,3,36HTARGET SURFACE-DISTANCE IN ANGSTROMS)
CALL LETTER (9,12,0,12,5,7,ANGSTROMS)
DO 51 JAB=1,5
CDC=FLOAT(JAB)*2*C0
XP=FLOAT(2+JAB)+1.6
YP=1.7
ENCODE (10,76,BCD) CDC
CALL LETTER (4,12,0,XP,YP,BCD)
CONTINUE
DO 52 JAB=1,5
CDC=FLOAT(JAB-1)*C0
XP=1.25
YP=4.5*FLOAT(JAB-1)
ENCODE (14,76,BCD) CDC
CALL LETTER (4,12,0,XP,YP,BCD)
CONTINUE
DO 53 JAB=1,4
CDC=FLOAT(JAB)*C0
XP=1.25
YP=4.5*FLOAT(JAB-1)
ENCODE (14,76,BCD) CDC
CALL LETTER (4,12,0,XP,YP,BCD)
CONTINUE
CALL LETTER (19,2,10,75,9,25,19HDAMAGE DISTRIBUTION)
CALL LETTER (14,12,1,3,9,14, INTERSTITIAL)
CALL LETTER (9.12,0,3,8.75,9HO VACANCY)
CALL LETTER (16,12,0,3,8,5,16HY FINAL POSITION)
CALL LETTER (16,12,0,3,8,25,16M OF THE PRIMAR)
CALL PLOT (2,5,5,3)
JW=JW-1
CO=1+CO
NOUT=0
NOUT=0
DO 59 IL=1,JJ
XP=Z(IL)+COC
YP=Y(IL)+COC
XP=XP+Z
YP=YP+5
IF (YP.GT.10..AND.YP.LT.10.) GO TO 54
NOUT=NOUT+1
GO TO 58
CONTINUE
IF (XP.GT.1..AND.XP.LT.13.) GO TO 55
CONTINUE
IF (ICOD(IL).NE.9) GO TO 56
CALL LETTER (1,1,0,.XP,YP,1H)
GO TO 58
CONTINUE
IF (ICOD(IL).NE.10) GC TO 57
CALL LETTER (1,1,0,.XP,YP,1M0)
GO TO 58
CONTINUE
IF (ICOD(IL).NE.2) GO TO 58
CALL LETTER (1,1,0,.XP,YP,1HY)
CONTINUE
WRITE (5,77) NOUT,HOUT
CONTINUE
IF (KJ.NE.1.OR.IJ.NE.1) GC TO 61
CALL PLOT (11,0,+3)
CALL PLOT (-11,0,+99)
CONTINUE
JJ=J-1
DO 62 I=1,JJ
XX=0
ZZ=0
STRX=0
STRY=0
STRZ=0
CONTINUE
KN=0
DO 64 I=1,JJ
IF (ICOD(I).EQ.9) GO TO 63
KN=KN+1
XX=XX+X(I)
YY=YY+Y(I)
ZZ=ZZ+Z(I)
STRX=STRX+X(I)*X(I)
STRY=STRY+Y(I)*Y(I)
STRZ=STRZ+Z(I)*Z(I)
CONTINUE
IF (IJ.GT.ML) GO TO 64
CALL PLOTP (Z(I),X(I),ICCD(I))
CONTINUE
XX=XX/KN
YY=YY/KN
ZZ=ZZ/KN
STRX=STRX/KA
STRY=STRY/KA
STRZ=STRZ/KA
STRX=SQR(STRX-XX*XX)
STRZ=SQR(STRZ-ZZ*ZZ)
YA=YA+YY
ZAX=ZA+ZZ
XAZ=XAZ+STRX
YA=YA+STRY
ZAZ=ZAZ+STRZ
IF (IJGTML) GO TO 65
CALL OUTPUT
CALL PRINTW (9HX VERS. Z)
CALL OUTLIN
CONTINUE
65 IF (IJGTML) GO TO 67
DO 66 I=1,IJ
CALL PLOTP (Z(I),Y(I),ICCD(I))
CONTINUE
CALL OUTPUT
CALL PRINTW (9HY VERS. Z)
CALL OUTLIN
CONTINUE
DO 68 I=1,IV
FN(IJ,I)=FN(IJ,I)+FLOAT(NDP(I))
CONTINUE
CONTINUE

******************************************************************************
* AVERAGING THE OUTCOME OF THE MOTION OF M PARTICLES
******************************************************************************

OUTPUT RESULTS.

DDE=DDE/FLOAT(M)
ITP=1
DO 70 J=1,IV
DO 72 I=1,IV
IF (FD(IJ).LT.FF) GO TO 72
FF=FD(I)
CONTINUE
70 CONTINUE
FF=1*FF
ITP=ITP+1
DO 72 I=1,IV
FL=FD(I)/100.*FF
CALL PLOTP (DE(I),FL,4)
CONTINUE
72 CONTINUE
IF (FD(IJ).LT.FF.OR.I.EQ.IV) GO TO 75
FL=FD(I)/100.*FF
CONTINUE
CALL PLOTPT (DE(I),FL.4)
STOP
75
76 FORMAT (2E14.4)
77 CONTINUE
78 CALL OUTPLT
79 CALL PRINTW (19Hdamage distribution)
80 CALL OUTLIN
81 XA=XA/M
82 YA=Y'A/M
83 ZA=ZA/M
84 XA2=XA2/M
85 YA2=YA2/M
86 ZA2=ZA2/M
87 WRITE (6,92) XA
88 WRITE (6,93) YA
89 WRITE (6,94) ZA
90 WRITE (6,95) XA2
91 WRITE (6,96) YA2
92 WRITE (6,97) ZA2
93 WRITE (6,98) kW
94 WRITE (6,99)�
95 WRITE (6,101) RATIO
96 STOP
97 C
98 FORMAT (F5.0)
99 FORMAT (15HNumber of reflected particles:***14)
100 FORMAT (15Hsurface penetration depth normal to the substrate:***14)
101 FORMAT (15Haverage penetration depth along another perpendicular direction:***14)
102 FORMAT (15Hthe straggling along the first direction:***14)
103 FORMAT (15Hthe straggling along the second direction:***14)
104 FORMAT (15Hprimary NC:***2x**4x**4x**4x)**
105 FORMAT (15HMCN CARLO ANALYSIS FOR RANGE CALCULATIONS:***15)
106 FORMAT (15HTotal range distribution:***10(15x,14)
107 FORMAT (15Hdeposited energy distribution:***15)
108 FORMAT (15Htotal deposited energy:***10(15x,14)
109 FORMAT (15Hthe average along the X axis is:***10(15x,14)
110 FORMAT (15Hthe average along the Y axis is:***10(15x,14)
111 FORMAT (15Hthe straggling along the X axis is:***10(15x,14)
112 FORMAT (15Hthe straggling along the Y axis is:***10(15x,14)
113 FORMAT (15Hthe total number of displaced atoms is:***10(15x,14)
114 FORMAT (15Htotal number of collisions is:***10(15x,14)
115 FORMAT (15H20x,24(*)+***10(15x,14)
116 FORMAT (2x,20x,24(*)+***10(15x,14)
104 IF8.2,1/
105 FORMAT ('/20X,MASS OF THE TARGET ATOMS',23(*,F10.2),/1/
106 FORMAT ('/20X,THE ELECTRONIC LOSS CONSTANT (K)*16(*,F8.2),/1/
107 FORMAT ('/20X,NUMBER OF INCIDENT PARTICLES*18(*,F14.4),/1/
108 FORMAT ('/20X,NUMBER OF INTERVALS PLOTTED*21(*,F8.2),/1/
109 FORMAT ('/20X,WIDTH OF EACH INTERVAL*21(*,F8.2),/1/
110 FORMAT ('/20X,INCIDENT ENERGY IN KEV*28(*,E16.8),/1/
111 FORMAT ('/20X,ELECTRONIC LOSS IS *2*E16.8**0.666667/E16.8),/1/
112 FORMAT ('/20X,CROSS-SECTION RATIO =*E16.8),/1/
113 FORMAT ('/20X,THE PROGRAM IS TERMINATED/**20X,THE NUMBER OF
114 FORMAT ('/20X,ADK',/1/
115 FORMAT ('/20X,KU',/1/
116 FORMAT ('/6.3,F15.6),/1/
117 FORMAT ('/6.3,F12.6),/1/
118 FORMAT ('/6.3,E16.8),/1/
119 FORMAT ('/6.3,E16.8),/1/
120 FORMAT ('/6.3,E16.8),/1/
121 FORMAT ('/6.3,E16.8),/1/
122 FORMAT ('/6.3,E16.8),/1/
END
SUBROUTINE TAB1 (T,SIGMA,X)
EXTERNAL FBT
DIMENSION T(1), SIGMA(1), X(1000)

THE STOPPING CROSS SECTION IS NUMERICALLY INTEGRATED
BY GAUSS GAUSSIAN FROM VALUES OF THE VARIABLE (T)
BETWEEN 1 E-4 AND 1 E-3
T = REDUCED ENERGY = SIN(THETA)**2
= THE SCATTERING ANGEL IN C.P. COORDINATES.

XO=ALOG(10000.),
M=X0/(N10-1)
T(1)=.0001
SIGMA(1)=0.
DO 1 T=10,1,10
1 T=EXP(-X(1))
U=1.(I)
UL=T(I-1)
CALL G08 (UL,UU,FBT,Y)
SIGMA(I)=SIGMA(I-1)+Y
CONTINUE
N12=200
XO=ALOG(1000.),
M=X0/(N12-1)
DO 2 I=1,N12
X(I)=*FLOT(I)
Y(I)=EXP(X(I))
**THE STOPPING CROSS SECTION INTEGRAL**

C = X**2 (4*9)
A = X**2 (-4/3)
B = 8.019
FBT = A/B
RETURN

SUBROUTINE LOCATE (THC,PHC,TH1,PH1,TH2,PH2,EL,EE,TK,X0,YO,ZO,J1,IC
1,ALL,IC,TKO,ITYP,AM1,AM2,FAI,THET,TIM,X,Y,Z,U,P,DE,NDP,DEC,NN,I
2,DL,DLL)
DIMENSION X(1), Y(1), Z(1), THET(1), FAI(1), B(3,3), A1(3,3), A2(3
1,3), E2(3,3), DP(1), CPT(1), DE(1), NDP(1)
COMMON /B12/ IC
COMMON /B67/ EP,IN,JO
COMMON /B77/ NOP

**THIS SUBROUTINE PROJECTS THE DISTANCE TRAVELLED BETWEEN**
**SUCCESSIVE COLLISIONS ON THE LABORATORY AXES.**
**THE SCATTERING ANGLES OF THE RECOILS ARE STORED IN THE**
**ARRAY (THET). THE TIME OF A PARTICULAR EVENT IS STORED IN**
**AN ARRAY (TIM). THE COORDINATES OF THE RECOILS ARE STORED IN ARRAYS**
**(X, Y AND Z).**

IF (ITYP .EQ. 2)
IF (ITYP .EQ. 1)
IF (ICALL .NE. 1) GO TO 9

**PROJECTION OF THE DISTANCE TRAVELLED BY THE PRIMARY OR**
**THE RECOILS FOR THE FIRST COLLISION.**

X(J1) = X0 + SIN(TH0)*SIN(PHC)*EL
Y(J1) = Y0 + SIN(TH0)*COS(PHC)*EL
Z(J1) = Z0 + COS(TH0)*EL
IF (Z(J1) .LT. 0.0) GO TO 1
IQ = 1
RETURN
CONTINUE
B(1,1) = COS(PH0)
B(2,1) = -SIN(PH0)
B(3,1) = 0
B(1,2) = COS(TH0) * SIN(PH0)
B(2,2) = COS(TH0) * COS(PH0)
B(3,2) = -SIN(TH0)
B(1,3) = SIN(TH0) * SIN(PH0)
B(2,3) = SIN(TH0) * COS(PH0)
B(3,3) = COS(TH0)
A1(1,1) = COS(PH1)
A1(2,1) = -SIN(PH1)
A1(3,1) = 0
A1(1,2) = COS(TH1) * SIN(PH1)
A1(2,2) = COS(TH1) * COS(PH1)
A1(3,2) = -SIN(TH1)
A1(1,3) = SIN(TH1) * SIN(PH1)
A1(2,3) = SIN(TH1) * COS(PH1)
A1(3,3) = COS(TH1)
IF (NN. EQ. 1.AND.NCP. NE. 1) GO TO 5
A2(1,1) = COS(PH2)
A2(2,1) = -SIN(PH2)
A2(3,1) = 0
A2(1,2) = COS(TH2) * SIN(PH2)
A2(2,2) = COS(TH2) * COS(PH2)
A2(3,2) = -SIN(TH2)
A2(1,3) = SIN(TH2) * SIN(PH2)
A2(2,3) = SIN(TH2) * COS(PH2)
A2(3,3) = COS(TH2)
DO 4 I = 1, 3
DO 3 J = 1, 3
S = 0.
DO 2 K = 1, 3
S = S + B(I,K) * A2(K,J)
CONTINUE
B2(1,J) = S
CONTINUE
AD = SQRT(B2(1,3) * B2(1,3) + B2(2,3) * B2(2,3))
THE(J) = ATAN(A4 / B2(3,3))
FAI(J) = ATAN(B2(1,3) / B2(2,3))
CONTINUE
DO 8 I = 1, 3
DO 7 J = 1, 3
S = 0
DO 6 K = 1, 3
S = S + B(I,K) * A1(K,J)
CONTINUE
B(I,J) = S
CONTINUE
CONTINUE
GO TO 18

**************************************************************
* PROJECTION OF THE DISTANCE TRAVELLED BY THE PRIMARY OR *
* THE RECOILS FOR SUBSEQUENT COLLISIONS.                  *
**************************************************************

CONTINUE
A1(1,1) = COS(PHI1)
A1(2,1) = SIN(PHI1)
A1(3,1) = 0
A1(1,2) = COS(THI1) * SIN(PHI1)
A1(2,2) = COS(THI1) * COS(PHI1)
A1(3,2) = SIN(THI1)
A1(1,3) = SIN(THI1) * SIN(PHI1)
A1(2,3) = SIN(THI1) * COS(PHI1)
A1(3,3) = COS(THI1)
IF (NN = EQ.1 AND NCPR * NE.1) GO TO 13
A2(1,1) = COS(PHI2)
A2(2,1) = SIN(PHI2)
A2(3,1) = 0
A2(1,2) = COS(THI2) * SIN(PHI2)
A2(2,2) = COS(THI2) * COS(PHI2)
A2(3,2) = SIN(THI2)
A2(1,3) = SIN(THI2) * SIN(PHI2)
A2(2,3) = SIN(THI2) * COS(PHI2)
A2(3,3) = COS(THI2)
DO 12 I=1,3
DO 11 J=1,3
S=0.
DO 10 K=1,3
S=S+B(I*K) * A2(K,J)
10 CONTINUE
B2(1+J)=S
11 CONTINUE
CONTINUE
AD=SQR(B2(1,3) * B2(1,3) + B2(2,3) * B2(2,3))
THET(JJ1)=ATAN(AD/B2(2,3))
FAI(JJ1)=ATAN(B2(1,3)/B2(2,3))
12 CONTINUE
X(JJ1)=X(JJ1-1)+B(1,3) * EL
Y(JJ1)=Y(JJ1-1)+B(2,3) * EL
Z(JJ1)=Z(JJ1-1)+B(3,3) * EL
IF (Z(JJ1) * GT * 0.) GO TO 14
13 RETURN
CONTINUE
DO 17 J=1,3
DO 16 L=1,3
S=0.
DO 15 K=1,3
S=S+B(I*K) * A1(K,J)
15 CONTINUE
B(I,J)=S
16 CONTINUE
CONTINUE
17 CONTINUE
CONTINUE
IF (NUP GT 6) GO TO 21
DO 20 JIK=1,1M
ZZ=Z(JJ1)
IF (ZZ LT * DE(JIK) OR ZZ GE DE(JIK+1)) GO TO 14
IF (J0 = EQ.1) GO TO 19
IF (TK GE EKIN) GC TO 20.
DP(JIK)=DP(JIK)+TK
IF (TK LT 50.) DPL(JIK)=DPL(JIK)+TK
GO TO 20
CONTINUE
DP(JIK)=DP(JIK)+TK
20 CONTINUE
GO TO 21
IF (TK.LT.50.) DPL(JIK)=DPL(JIK)+TK
CONTINUE
IF (NCP.EQ.1) RETURN
DO 22 I=1,IM
ZZ=Z(JI)
IF (IZZ.LT.1) ZZ=ZZ+DLL
DP(I)=DP(I)+TK
IF (TK.GT.25.) NCP(I)=NCP(I)+1
IF (TK.LT.50.) DPL(I)=DPL(I)+TK
CONTINUE
RETURN
END

SUBROUTINE FOLLOW (IH1, IH2, PH1, PH2, EL, J1, ITYP, T, SIGMA1, T1, SIGMA2, E, AL1, AL2, AK1, AK2, GAMA)

AL1=AK1(ITYP)
AL2=3.*AK3(ITYP)
A3=AK3(ITYP)
A3=18.334*A3
TMAX=A1**EV*EV*GAMA*GAMA
THIN=AL1**EV*25.
ICO=0
CONTINUE
CA=0.01*CC(ITYP)
CA=1.E-6*CC(ITYP)

AN APPROXIMATION OF THE STOPPING CROSS SECTION WITH A
POWER CROSS SECTION WITH (M=0).

IB=0
IF (EV.GT.CA) GO TO 2
TMAX=GAMA*GAMMA*EV
SIGMA=AS*ALOG(TMAX)
TS=TMAX**25.
IF (EV.GT.CA) GO TO 2
IB=1
GO TO 34

DIMENSION SIGMA1(1), T1, SIGMA2, E, AL1, AL2, AK1, AK2, GAMA
COMMON /TYP/ CON
COMMON /ST/ NCP
COMMON /BE/ MOP
CONTINUE
TH=THMIN**(-1.0/3.)
TX=THMAX**(-1.0/3.)
IF (THMAX.LT.1300.) GO TO 3
WRITE (6,43)
CALL EXIT
CONTINUE

******************************************************************************
* AN APPROXIMATION OF THE STOPPING CROSS SECTION WITH A *
* POWER CROSS SECTION WITH (M=1.0/3.). *
******************************************************************************

IF (THMAX.GT.0.001) GO TO 4
SIGMAT=A2*(TH-THX)
SIGMAV=Q1*SIGMAT
TA=(1.0-Q1)*TH
TB=Q1*TH
TB=TA*TB
TA=TA**3
TS=1./TA
GO TO 34

******************************************************************************
* THIS PART IS CALCULATED BY NUMERICAL INTEGRATION *
******************************************************************************

CONTINUE
IF (THMIN.LT.0.001) GO TO 18
DO 11 KK=1,2
IF (KK.EQ.1) TV=THMIN
IF (KK.EQ.2) TV=THMAX
J=10
I=1
5 IF (TV.GT.T(J)) GC TO 6
GO TO 7
6 I=I+1
J=J+10
GO TO 5
CONTINUE
IF (J.NE.10) GO TO 9
JJ=1
DO 8 K=1,10
AS=ABS(TV-T(K))
BS=ABS(TV-T(JJ))
IF (AS.LT.BS) JJ=K
8 CONTINUE
SIGMA(KK)=SIGMAN(JJ)
GO TO 11
CONTINUE
LL=J-10
LU=J
JJ=1
DO 10 K=LL+1,LU
AS=ABS(TV-T(K))
BS=ABS(TV-T(JJ))
10 CONTINUE
IF (AS.LT.BS) JJ=K
CONTINUE
SIGMA(KK)=SIGMAN(JJ)
CONTINUE
SIGMAT=SIGMA(2)-SIGMA(1)
SIGNAV=SIGMAT*Q1+SIGMA(1)
J=10
I=1
IF (SIGNAV.GT.SIGMAN(J)) GO TO 13
GO TO 14
I=I+1
J=J+10
GO TO 12
CONTINUE
IF (J.NE.10) GO TO 16
JJ=1
DO 15 K=1,10
AS=ABS(SIGMAV-SIGMAN(K))
BS=ABS(SIGMAV-SIGMAN(JJ))
IF (AS.LT.BS) JJ=K
15 CONTINUE
TS=T(JJ)
SIGMAT=SIGMAT*A3
GO TO 34
CONTINUE
LL=J-10
LU=J
JJ=1
DO 17 K=LL,LU
AS=ABS(SIGMAV-SIGMAN(K))
BS=ABS(SIGMAV-SIGMAN(JJ))
IF (AS.LT.BS) JJ=K
17 CONTINUE
TS=T(JJ)
SIGMAT=SIGMAT*A3
GO TO 34
CONTINUE
SIGMA(1)=A2*(TH-21.54)
J=10
19 IF (TMAX.GT.T(J)) GC TO 20
GO TO 21
I=I+1
J=J+10
GO TO 19
CONTINUE
IF (J.NE.110) GO TO 23
JJ=1
DO 22 K=1,10
AS=ABS(TMAX-T(K))
BS=ABS(TMAX-T(JJ))
IF (AS.LT.BS) JJ=K
22 CONTINUE
SIGMA(2)=SIGMAN(JJ)*A3
GO TO 25
CONTINUE
LL=J-10
LU=J
JJ=1
DO 24 K=LL,LU
\[ \text{AS} = \text{ABS}(\text{TMAX} - T(K)) \]
\[ \text{BS} = \text{ABS}(\text{TMAX} - T(JJ)) \]
\[ \text{IF} (\text{AS} \cdot \text{LT} \cdot \text{BS}) \quad J = K \]
\[ \text{CONTINUE} \]
\[ \text{SIGMA}2 = \text{SIGMAN}(JJ) \cdot \text{A3} \]
\[ \text{CONTINUE} \]
\[ \text{SIGMA}1 = \text{SIGMA}(1) \cdot \text{SIGMA}(2) \]
\[ \text{SIGMA}V = \text{Q1} \cdot \text{SIGMA}1 \]
\[ \text{IF} (\text{SIGMA}V > \text{SIGMA}(1)) \quad \text{GO TO 27} \]
\[ \text{TS} = 1.0 - (\text{TP} - (\text{SIGMA}V / \text{A2})) \cdot 0.3 \]
\[ \text{IF} (\text{TS} \cdot \text{GT} \cdot 0.0) \quad \text{GO TO 26} \]
\[ \text{WRITE} (C \cdot 42) \]
\[ \text{CONTINUE} \]
\[ \text{GO TO 34} \]
\[ \text{CONTINUE} \]
\[ \text{SIGMA}V = \text{SIGMA}V - \text{SIGMA}(1) \]
\[ \text{SIGMA}V = \text{SIGMA}V / \text{A3} \]
\[ J = 10 \]
\[ I = 1 \]
\[ \text{IF} (\text{SIGMA}V > \text{SIGMA}(J)) \quad \text{GO TO 29} \]
\[ \text{GO TO 30} \]
\[ I = I + 1 \]
\[ J = J + 10 \]
\[ \text{GO TO 28} \]
\[ \text{CONTINUE} \]
\[ \text{IF} (J \cdot \text{NE} \cdot 10) \quad \text{GO TO 32} \]
\[ J = 1 \]
\[ \text{DO} 31 \quad K = 1 : 10 \]
\[ \text{AS} = \text{ABS}(\text{SIGMA}V - \text{SIGMA}(K)) \]
\[ \text{BS} = \text{ABS}(\text{SIGMA}V - \text{SIGMA}(JJ)) \]
\[ \text{IF} (\text{AS} \cdot \text{LT} \cdot \text{BS}) \quad \text{JJ} = K \]
\[ \text{CONTINUE} \]
\[ \text{TS} = T(JJ) \]
\[ \text{GO TO 34} \]
\[ \text{CONTINUE} \]
\[ LL = J - 10 \]
\[ LU = J \]
\[ \text{DO} 33 \quad K = LL : LU \]
\[ \text{AS} = \text{ABS}(\text{SIGMA}V - \text{SIGMA}(K)) \]
\[ \text{BS} = \text{ABS}(\text{SIGMA}V - \text{SIGMA}(JJ)) \]
\[ \text{IF} (\text{AS} \cdot \text{LT} \cdot \text{BS}) \quad \text{JJ} = K \]
\[ \text{CONTINUE} \]
\[ \text{TS} = T(JJ) \]

**********THE SCATTERING ANGELS TH1 AND TH2**********
**********THE AZIMUTHAL ANGELS PH1 AND PH2**********

\[ \text{CONTINUE} \]
\[ \text{IF} (I(G) \cdot \text{EC} \cdot 1) \quad \text{GO TO 38} \]
\[ \text{RA} = \text{TS} / \text{TMAX} \]
\[ \text{IF} (\text{RA} \cdot \text{LT} \cdot 1.0) \quad \text{GO TO 35} \]
\[ \text{TS} = \text{TMAX} \]
\[ \text{TH1} = 0.0 \]
\[ \text{TH2} = 0.0 \]
\[ \text{GO TO 36} \]
CONTINUE
TH2=ASIN(SQRT(RA))
TH1=AL(ITYP)*SINV/(1.*AL(ITYP)*COS(TH))
TH =ATAN(TH2)
TH2=ATAN(TH1)
CONTINUE
PH1=6.28*C2
PH2=(2*C1/7.)*PH1
TK=TS/(1)*EV
IF (I9=EQ.1) TK=TS
GO TO 37
CONTINUE
E(J1)=TK

* CALCULATION OF THE DISTANCE BETWEEN SUCCESSIVE COLLISIONS *

AC=AL(ITYP)
IF (Q3=EQ.0.) Q3=1.E-3
EL=CON ALOG(Q3)/SIGMAT
IF (EL=LT.2.7) EL=2.7

* ELECTRONIC LOSS (DEC) *

CONTINUE
IDL=0
IF (N0P.EQ.0) GO TO 80
IF (NN.EQ.0) GO TO 80
IF (TK.LT.60) GO TO 80

THMIN=.025
THMAX=.1625
IF (ICO.EQ.1) GO TO 39
ICO=1
GO TO 1
CONTINUE
ELL=CON ALOG(Q3)/SIGMAT
DLL=ELL*CCS(TH2)
IDL=1
CONTINUE
CW=EL/(2.*VA2(ITYP))
DEC=EV-(SQR(EV)-Ch)**2
LMAX=2.*VA2(ITYP)*SQR(EV)
IF (EL.EQ.LMAX) GO TO 43
DEC=EV-TK
EL=LMAX
CONTINUE
DDE=DDE-DEC
RETURN

FORMAT (/,* MU N2 *8)
FORMAT (/,* THE VALUE OF T IS GREATER THAN 1000. *8,/)