ESTIMATION OF THE AVERAGE ENERGY DISSIPATED IN ELASTIC COLLISIONS BY THE PRIMARY KNOCK-ONS PRODUCED IN NEUTRON IRRADIATION

by

Anthony Robin Fallon

A Thesis Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
MASTER OF SCIENCE

Major Subject: Nuclear Engineering

Signatures have been redacted for privacy

Iowa State University
Of Science and Technology
Ames, Iowa

1963

TABLE OF CONTENTS

INTRODUCTION

The major direct result of neutron irradiation on a solid is the creation of interstitial-vacancy pairs in the ordered structure of a substance as a result of elastic collisions between the neutrons and stationary atoms. The damage from the displacement production is directly noticed in changes in the electrical, thermal and elastic properties in an irradiated solid. The atoms displaced by neutrons, called primary knock-ons, may also displace stationary atoms by atomic collisions. Although it has been suggested that some vacancies may come from ionization (12) essentially all the displacements are caused by elastic collisions with the stationary atoms and the neutrons or the knock-ons.

The moving neutrons and displaced atoms, however, are responsible for effects other than vacancy-formation. A neutron can also cause impurities in a substance by transmutation of a nucleus that has captured it, but this reaction may be neglected when compared to elastic collisions (9). Since the primary knock-on is a charged particle there exists a competition for its energy between the processes of elastic collisions with other atoms and inelastic collisions with electrons. Ionization and electronic excitation predominate when the particle has a high velocity and is stripped of all its orbital electrons. At slower speeds the knock-on becomes a neutral atom by regaining its electrons and then favors elastic collisions.

The total number of displacements formed in the target material by the neutron beam is generally determined by finding the number of primary knock-ons formed by the neutrons and multiplying this number by the average number of displacements per primary. The number of knock-ons is relatively easy to find if the neutron flux and the scattering cross section of the target material are known. Calculating the number of displacements per primary, however, is complicated by the close competition between elastic and inelastic interactions. The number of displacements formed in a solid is proportional to the energy that the primary knock-on loses in elastic collisions.

The methods used to determine the energy lost in elastic collisions by a charged particle are generally based on gross simplifying assumptions. A large part of the energy that goes to elastic collisions is neglected by assuming there exists a threshold energy above which the knock-on may participate only in inelastic collisions. There is a need for a more accurate determination of the energy lost in elastic collisions by the primary knock-ons resulting from neutron irradiation because these collisions are responsible for most radiation damage. The purpose of this paper is to attempt to fulfill this need.

The procedure for finding the energy lost in elastic collisions to be used here is too cumbersome for everyday use whenever this quantity must be known. In order to make the results of this investigation useful, therefore, the values of the energy lost in elastic collisions were tabulated and plotted against initial neutron energy for the elements considered here. From these tables and graphs a general empirical equation was found that relates the energy lost in elastic collisions to the initial neutron energy and to the atomic number of the target material.

REVIEW OF LITERATURE

Early interest in energy loss of radiation in matter was centered around alpha-particles in air. Calculations of stopping power, or energy loss per unit path length, as outlined by Livingston and Bethe (20) considered only the inelastic electron encounters. It was recognized that for stopping of high speed particles in a gas or light solid, ionization and electron excitation were responsible for nearly all of the energy loss. Range versus energy curves were thus plotted on this assumption of only inelastic collisions. The primary concern of these studies was the radiation itself rather than the stopping materials and these range-energy graphs were primarily used to determine the initial energy of a particle stopped after traveling a known distance in a substance.

With the discovery of nuclear fission and the ensuing possibility of radiation damage to materials in or near the "atomic piles" the interest began to shift from the effect on the incoming particles to the damage caused by the radiation in the target material. E. P. Wigner in 1942 considered the result of fast neutrons impinging on a solid and showed theoretically the occurance of displacements (10). Most of the work in this area that was done during the Second World War was shrouded in secrecy and post-War progress was slowed until the work was generally declassified.

Niels Bohr headed a group in Copenhagen working on the general field of atomic particle penetration and published a complete coverage of the field up to that time in 1948 (5). Although the primary concern of this paper was the interaction of atomic particles with gases much of Bohr's results are applicable to solids and his work has served as a vital reference for virtually every subsequent study. He considered separately the effects of elastic collisions, inelastic collisions and found the combined total stopping expressions for various energy ranges of particles and various atomic weights of stopping materials.

Frederick Seitz in 1949 presented a comprehensive survey of disordering of solids by massive particles (24) concerned with determining the number of displacements caused by different radiations. He obtained values for the number of displacements formed in Be, C, Al, Si, and Ge irradiated with alpha-particles, protrons and neutrons. To find the number of displacements he first had to weed out the energy lost due to ionization and electron excitation. The energy lost due to elastic collisions by a charged particle was thus found by assuming a threshold energy E_i such that only elastic collisions can occur if the particle has kinetic energy less than E_i. If a moving atom, however, has energy greater than E_i the energy loss is divided between elastic and inelastic interactions. The energy lost to elastic collisions as a function of primary knock-on kinetic energy T will be called G(T). Seitz then used

$$G(T) = T, \qquad T \leq E_i \qquad (1a)$$

$$G(T) = T + \left[(T - E_i) \frac{(dT/dx)_c}{(dT/dx)_i}\right], \qquad T \geq E_i \qquad (1b)$$

where $(dT/dx)_c$ is the energy lost to elastic collisions per unit path length dx and $(dT/dx)_i$ is the energy lost to inelastic collisions per unit path length.

The threshold energy E_i is treated differently for metals and non-metals. For insulators there will be essentially no interaction with the charged particle and the orbital electrons if the velocity of the moving particle is small with respect to the velocity of the slowest orbital electron. For insulators Seitz suggests that

$$E_i = \frac{M}{m_e} \frac{E_e}{8} \tag{2}$$

where M is the atomic mass of the stopping material, m_e is the electronic mass, and E_e is the lowest electronic excitation energy for the insulator.

The electronic collision cut-off is not too well defined for metals because the free electrons, unlike orbital electrons, can have arbitrarily low velocities. Seitz treats the case for metals by taking E_i as that energy for which the energy losses of the moving atom are equal for elastic and inelastic collisions, i.e., when $(dT/dx)_c = (dT/dx)_i$.

Seitz's treatment leads to several objections. First of all, the use of a sharp threshold E_i is not strictly valid, particularly for metals, since there can still be electronic encounters for $T < E_i$. The value of E_i chosen for metals is somewhat arbitrary and cannot be expected to give better results than just proper order of magnitude. The main drawback, however, lies in his assumption that the ratio of energy lost elastically to energy lost inelastically is equal to a constant value of the order of 10^{-3}. This assumption is poor except for very high energies where this ratio is nearly constant and T is large with respect to E_i. The very definition of E_i for metals requires that R = 1 at E_i which is contrary to the above assumption.

Burton, earlier, had mentioned the existance of a "threshold energy" above which electronic excitation was prominent and below which the elastic collisions prevailed. He pointed out, though, that "The threshold .... is by no means sharp" (10). Most of the subsequent studies, however, have relied upon a definite threshold E_i in order to determine G(T). Brinkman (6) used an approximation for E_i such that

$$E_i = \frac{M}{m_e} E_{ion} \qquad (3)$$

where E_{ion} is the "ionization energy of the atom" and was assumed to be 5 electron volts for all elements. The value of E_i used by Holmes (14) has the same form as Equation 3 with E_{ion} taken as 2 ev. The two estimations given above made no distinction between metals and non-metals. Although in agreement with the value of E_i used by Seitz (24) for insulators, Kinchin and Pease (16) took exception to his rather arbitrary cut-off used for metals. Assuming that when the velocity of the moving atom is much less than the most energetic of the conduction electrons there will be few electrons excited, the value of E_i for metals is taken to be

$$E_i = \frac{M}{m_e} \frac{\epsilon_o}{16} \qquad (4)$$

where ϵ_o is the Fermi energy of the free electrons. Values of E_i are given for most metals that are intended to represent the limit below which ionization losses may be neglected (Table 2.3, 16).

Dienes and Vineyard (12) suggested a "rule of thumb" for estimating the ionization threshold E_i. The lowest electronic excitation energy, E_e in Equation 2, is around 5 ev for most insulators. Most metals have a fermi energy ϵ_o of the order of 2 to 12 ev. Equations 2 and 4 then both give a common value of $E_i \approx (M/m_e)/2$. For insulators and metals, therefore, E_i, in kev, is approximately equal to the atomic mass number A of the targe element.

The value of G(T) given by Kinchin and Pease (16) for $T > E_i$ is admitted to be essentially the same as Equation 1b. However, if T is not greatly in excess of E_i, they decided, "....it is often sufficient to suppose that all excess energy is expended in ionization losses.." In other words, they used the threshold energy to hold for both elastic and inelastic collisions.

Snyder and Neufeld, (26) considering the disordering of solids caused by neutron irradiation, decided that the energy of primary knock-ons lost in elastic collisions could be represented as follows:

$$G(T) = T \qquad T \leq E_i \qquad (5a)$$

$$G(T) = E_i \qquad T \geq E_i. \qquad (5b)$$

Justification for neglecting much of the energy lost in elastic encounters was that the probability of an elastic collision for $T > E_i$ was considered to be very small. Dienes (11) and Seitz and Koehler (25) likewise assumed that the maximum energy that can go into elastic collisions is given by that energy for which electron excitation ceases, i.e., E_i for high-speed, charged particles.

Hurwitz and Clark suggested a method for finding the energy dissipated in elastic collisions which was presented by Bruch, et al. (9). The ratio of stopping power due to elastic collisions to total stopping power for primary knock-ons resulting from neutron irradiation is designated f(T), i.e.

$$f(T) = \frac{(dT/dx)_c}{(dT/dx)_t} = \frac{(dT/dx)_c}{(dT/dx)_c + (dT/dx)_i} \tag{6}$$

The function f(T), therefore, represents the fraction of energy lost by a knock-on that goes into elastic collisions. For a small increment of primary knock-on energy dT the part of the energy that is expended in elastic collisions is dG = f(T)dT. Then if a charged particle has initial energy T and loses all this energy passing through a solid, the energy G(T) lost to elastic collisions is

$$G(T) = \int_0^T f(T)\, dT \tag{7}$$

The above relationship holds only for one or more charged particles all having energy T. In neutron bombardment, however, the primary knock-ons will have all values of energy in the range $0 \leq T \leq T_m$ even if all the neutrons have the same energy. The maximum possible energy transferred by neutrons of energy E to a stationary atom is given by

$$T_m = \frac{4A}{(1 + A)^2} E \tag{8}$$

where A is the atomic weight number of the target material.

Assuming the neutron scattering to be isotropic, Hurwitz and Clark averaged G(T) over the entire primary knock-on energy range to find the average energy lost in elastic collisions $\overline{G(E)}$ as a function of the neutron energy E:

$$\overline{G(E)} = \frac{1}{T_m} \int_0^{T_m} G(T)\, dT \qquad (9)$$

This procedure for finding $\overline{G(E)}$ was used by Hurwitz and Clark for only three elements Be, C, and Fe. The equations for stopping power in this study, however, were not truly applicable to all these substances and the energy ranges involved. For example, they took their expression for the rate of energy loss due to elastic collisions to apply over the entire range, but the equation is actually only good for very high energies. Also, the $(dT/dx)_i$ terms they used for all their elements are meant to be used for metals only.

The estimates of the part of the energy lost by charged particles that goes into elastic collisions used in other studies are substantially the same as those mentioned and are thus not listed here.

PROCEDURE

The upper limit for the neutron energy in the following calculations was taken as 10 Mev. This limit is based on the fact that the average fast neutron energy in a nuclear reactor is of the order of 1 or 2 Mev and few neutrons have energies above 10 Mev. Since reactors are the only important source of neutrons, energies above this 10 Mev limit were not considered.

Only the lighter elements were considered here. In the energy range of interest the heavier elements will not have the competition between elastic and inelastic energy losses by the primary knock-ons because of the high value of the ionization threshold E_i. As the atomic mass increases E_i increases, and the maximum possible energy T_m transferred by a neutron to a stationary particle decreases, so that essentially all of the primary knock-on kinetic energy is lost in elastic collisions in heavy elements. For all elements heavier than iron a neutron energy of greater than 1 Mev is necessary before any inelastic collisions are possible.

The target elements were considered to be homogeneous, isotropic and monatomic solids. The atomic mass number A was taken as the average atomic weight for a natural isotropic mixture.

The general approach to the problem of determining the average energy $\overline{G(E)}$ lost in elastic collisions as a function of the initial neutron energy was similar to the procedure of Hurwitz and Clark (9) as outlined in the previous chapter. The fraction of energy $f(T)$ lost in elastic collisions was integrated over the entire primary knock-on energy range to find the portion $G(T)$ of energy T that goes into elastic collisions. Averaging $G(T)$ over the knock-on energy range then yields $\overline{G(E)}$ in terms of the neutron energy E.

In order to find $f(T)$ the rate of energy loss per unit path length (dT/dx) had to be determined for both elastic and inelastic collisions. The stopping of the primary knock-ons was assumed to be due to only these elastic and/or inelastic collisions. The stopping of the primary knock-ons was assumed to be due to only these elastic and/or inelastic collisions, i.e.

$$(dT/dx)_t = (dT/dx)_c + (dT/dx)_i \qquad (10)$$

where $-(dT/dx)_t$ is the total stopping power and the subscripts "c" and "i" refer to elastic and inelastic collisions respectively.

The stopping material was assumed to be monatomic. The significance of this assumption is that the knock-on will have encounters with atoms of the same mass and atomic number. A primary knock-on of energy T can then lose up to all its energy in a single elastic encounter.

Rate of Energy Loss $-(dT/dx)_c$ Due to Elastic Collisions

High energy range

An atom traveling at a high speed will have no electrons attached and will hence be a highly charged particle. A stationary atom, on the other hand, is surrounded by electrons which tend to screen the electrostatic potential of the nucleus. The high energy particle, however, penetrates the electron cloud and the two nuclei "see" each other unscreened. Then the interaction between the two is essentially that of two ions of charge Z e, where Z is the atomic number of the knock-on and the stationary atom, and e is the electronic charge. This brief period of unscreened interaction is the most important part of the particle's trajectory as far as scattering is concerned (14). Elastic collisions of high speed particles, therefore, can be treated as a Coulomb or Rutherford scattering problem.

The differential cross-section for Rutherford scattering (5) is given by

$$d\sigma_c = B_c \frac{dT'}{(T')^2} \tag{11}$$

where T' is the energy transferred from the moving atom to the stationary atom. For a case when both incident and target atom have the same mass and charge

$$B_c = 2\pi \frac{Z^4 e^4}{M v^2} \tag{12}$$

where M is the mass of the atom and v is the velocity of the moving particle.

The energy loss per unit path length, as given by Bohr (5), will then be

$$-(dT/dx)_c = N \int_{T'_s}^{T'_m} T' d\sigma \tag{13}$$

where N is the number of atoms per unit volume in the stopping material,

T'_s is the smallest possible energy transfer in a Rutherford collision, and T'_m is the maximum possible nergy transfer in a Rutherford collision.

The stopping power due to elastic collisions, found by integrating the right-hand side of Equation 13, is then

$$-(dT/dx)_c = N\ B_c\ \ \ln(T'_m/T'_s) \tag{14}$$

where ln is the natural logarithm. If the moving atom has kinetic energy T the maximum energy transfer will be equal to T, i. e, $T'_m = T$. Seitz (24, p. 273) found for the lower energy transfer limit

$$T'_s = 2.47\ Z^{2/3}\ \frac{m_e}{M}\ E_R \tag{15}$$

where m_e is the electronic mass and the Rydberg energy $E_R = 13.54$ ev. Generally T'_s is of the order of 10^{-2} ev. The ratio m_e/M can be given as $1/(1840A)$ where A is the atomic mass number of the solid.

The equation for loss of knock-on energy due to elastic collisions, substituting Equations 12 and 15 into Equation 14 and simplifying the terms, will then be

$$-(dT/dx)_c = \pi\ \frac{Z^4\ e^4}{T}\ N\ \ln(T\ 55A/Z^{2/3}) \tag{16}$$

Equation 16 is only valid for high-energy particles. The moving atom, as it slows down, will begin to collect electrons and thus reduce its effective charge. Also, as the knock-on loses energy it becomes less able to fully penetrate the electron cloud surrounding the stationary atom and the interaction of the two will no longer be of the pure Coulomb type.

The condition as given by Bohr for Equation 16 to hold, is

$$\frac{8\sqrt{2}\,\pi^2 e^4 \quad Z^{7/3} m_e}{T\,h^2} \ll 1 \tag{17}$$

where h is Planck's constant. Substituting values for the constants in Equation 17 gives the following condition for the validity of Equation 16

$$T \gg 77 \quad Z^{7/3} \tag{18}$$

where T is in electron volts.

When log $(dT/dx)_c$ as given by Equation 16 is plotted against log (T) the resulting curve can quite closely be approximated by a straight line when $T \gg Z^{2/3}/55A$, where T is in electron volts. For high energy knock-ons it is then fairly accurate to use

$$-(dT/dx)_c \quad = \quad C_c \quad T^{-\alpha} \tag{19}$$

where $(-\alpha)$ is the slope on the log-log graph and C_c is a constant given by the value of $(dT/dx)_c$ at log (T) = 0. The constants α and C_c were found graphically.

Intermediate energy range

In the intermediate energy range the moving ion and the stationary nucleus are partially screened with respect to one another and a simple Rutherford treatment no longer holds. The Coulomb potential between two unscreened nuclei is proportional to 1/r where r is the distance between the two.

For a partially screened electrostatic field Dienes and Vineyard (12) suggest that the interaction potential should be of the form

$$P(r) = \frac{Z^2 e^2}{r} \epsilon^{-r/a} \tag{20}$$

where P(r) is the interaction potential, ϵ is the base of natural logarithms, and a is a screening constant with the dimensions of length.

Earlier, however, Bohr (5) suggested that a screened potential could be expressed as proportional to $1/r^n$ and indicated that n should be approximately equal to 2. Lindhard (18) verified that $n = 2$ in Bohr's expression is in good agreement with experimental results; therefore the interaction potential in the partially screened field for a moving ion in the kev energy range was taken here to be proportional to $1/r^2$. For this $1/r^2$ potential the rate of energy loss $(dT/dx)_c$ due to elastic collisions is independent of energy.

Lindhard and Scharff used a differential cross-section for elastic scattering in the intermediate region that has the following form:

$$d\sigma_c = K \frac{dT'}{(T)^{3/2}} \tag{21}$$

As in the case of Rutherford scattering, Equation 21 gives a greater probability for small energy transfers.

The K in Equation 21 is constant with respect to the transfer energy T'. Lindhard and Scharff found that

$$K = \frac{\pi^2 e^2 a_o}{2\, \epsilon\, (T'_m)^{1/2}} \left(\frac{Z_1 Z_2}{\sqrt{Z_1^{2/3} + Z_1^{2/3}}} \right) \left(\frac{M_1}{M_1 + M_2} \right) \tag{22}$$

where T'_m is the maximum possible energy transfer from a moving atom to a stationary atom, the subscript "1" refers to the moving atom and the subscript "2" indicates the stationary atom, and a_o is the Bohr radius given by

$$a_o = \frac{h^2}{4\pi^2 m_e \, e^2} = 5.292 \times 10^{-9} \text{ cm} \qquad (23)$$

For the present case where the moving atom and the fixed atom are identical, i.e., $Z_1 = Z_2$ and $M_1 = M_2$, the energy transferred T' may vary between 0 and the primary knock-on energy T. The rate of energy lost to elastic collisions is then found by substituting Equation 21 into Equation 13 and integrating from 0 to T, yielding the following expression:

$$-(dT/dx)_c = \frac{h^2 \; Z^{5/3} \; N}{\sqrt{8} \;\; 2 \, m_e \, \epsilon} \qquad (24)$$

The value obtained by Bohr (5) for $(dT/dx)_c$ in the intermediate range was smaller than Equation 22 by the ratio $2/\pi$. The difference between the two treatments was that Bohr assumed isotropic scattering in a "hard-sphere" model. Equation 22 was preferred to Bohr's because it represents a less abrupt change in differential cross-section from the high-energy Rutherford collisions to the low energy hard-sphere collisions.

Low energy range

When the charged particles have low energies, below the kev range, the total elastic collision cross-section σ_c is independent of energy.

Both the moving and stationary atoms have all their electrons and the moving atom no longer has enough energy to penetrate the electron cloud; therefore, the interaction is essentially a collision between two neutral hard spheres.

The scattering for low energies is isotropic, i.e., all transfer energies are equally probable. The differential cross-section for this range is then given by

$$d\sigma_c = \sigma_c \frac{dT'}{T} \tag{25}$$

The stopping power for low energy elastic collisions is, therefore, from Equation 25 and Equation 13 with limits from 0 to T

$$-(dT/dx)_c = (1/2)\, N\, \sigma_c\, T \tag{26}$$

The value of $(dT/dx)_i$ for the low energy range was not determined here because here there is virtually no primary knock-on energy loss to inelastic collisions and $G(T) = T$.

Rate of Energy Loss $(dT/dx)_i$ Due to Inelastic Collisions

High energy range

Any ion moving at a high velocity will lose most of its energy in inelastic collisions. These collisions have been studied extensively both experimentally and theoretically. The stopping power due to inelastic interactions is given by the well-known Bethe-Bloch equation (20, p. 263)

$$-(dT/dx)_i = \frac{4\pi e^4 Z^3 N}{m_e v^2} \ln (2m_e v^2/I) \quad (27)$$

where I is the average excitation potential of the atom.

The average excitation potential is generally expressed as

$$I = I_o Z \quad (28)$$

where I_o is an empirical constant. Lindhard and Scharff (19) give a value of I_o = 10 ev based on experimental results.

The limitation of Equation 27 was given by Bethe and Ashkin (4) as

$$v \gg (2\pi Z e^2)/h \quad (29)$$

This restriction limits the equation to high-energy particles in light elements. For beryllium, the lightest element investigated, a primary knock-on energy of at least 4 Mev is needed for the condition of Equation 29 to be met. A beryllium atom needs a head-on collision with the maximum possible energy transfer from a 10 Mev neutron to gain this needed 4 Mev. Since 10 Mev was the maximum neutron energy considered here, Equation 27 was not used in the present calculations.

Intermediate energy range

As the charge of the primary knock-on decreases by virture of the slowing down process, there is less tendancy to have inelastic collisions with electrons. In the intermediate range, therefore, $(dT/dx)_i$ should decrease with the energy. Lindhard and Scharff (19) noted that the energy loss per unit path length of a charged particle of intermediate energy in an electron gas of constant density is proportional to the velocity. They also obtained the expression for $(dT/dx)_i$ in a later paper (18)

$$-(dT/dx)_i = \sqrt{2}\, a_o\, h\, N\, Z^{7/6}\, v \qquad (30)$$

Seitz (24) suggested an equation for $(dT/dx)_i$ in the intermediate and low energy range for metals. This expression gives $(dT/dx)_i$ proportional to the charged particle's energy. However, since Seitz admits the weakness of the assumptions behind his equation and since a metal with its free electrons is a good approximation to the electron gas of Equation 30, the equation of Lindhard and Scharff was used for both metals and non-metals.

Inelastic collision threshold energy E_i

If the velocity of an electron is less than the velocity of a primary knock-on the probability of the knock-on losing energy to the electron is very low. This means that in an insulator there will be essentially no inelastic electron encounters if the moving ion is not going as fast as the slowest orbital electrons. Therefore it was assumed that if a primary knock-on has energy less than E_i, as given by Equation 2, the energy loss will be due to only elastic collisions in a non-metal.

The conduction electrons in a metal have no lower energy limit and could therefore interact with very slow moving atoms. The encounter between the two, however, would be elastic since the free electrons cannot be excited to different energy levels as are orbital electrons. The energy loss to these electrons in metals will then be quite small due to the great mass difference between the electrons and the primary knock-ons. The threshold energy E_i as given by Equation 4 was thus used as the lower limit for inelastic collisions in metals.

The values of the lowest excitation energy E_e for insulators were taken from a table of critical potentials of an atom given by Francis (13).

The Fermi energy ϵ_o for metals is calculated from the equation given by Seitz (23)

$$\epsilon_o = (h^2/2m_e)\ (3n/8\pi)^{3/2} \tag{31}$$

where n is the number of conduction electrons per unit volume.

Fraction of Energy f(T) Lost Due to Elastic Collisions

The portion of primary knock-on energy dissipated in elastic collisions is given by Equation 6. This equation can be written as

$$f(T) = \frac{1}{1 + R} \tag{32}$$

where

$$R = \frac{(dT/dx)_i}{(dT/dx)_c} \tag{33}$$

Low energy range

When $T < E_i$ the inelastic energy loss is negligible with respect to the loss due to elastic collisions, i.e., $R \ll 1$ and therefore $f(T) = 1$.

Intermediate energy range

The rate of energy loss due to elastic collisions for moving atoms in the intermediate energy range when $T > E_i$ is given by Equation 24. The general form for $(dT/dx)_c$ in this energy range can then be written

$$-(dT/dx)_c = D_c \tag{34}$$

where D_c is a constant given by the right hand side of Equation 24. The upper limit of applicability of Equation 34 is called T_a, the energy for which Equation 16 equals Equation 24.

From Equation 30 the energy loss due to inelastic collisions is proportional to the particle velocity and $(dT/dx)_i$ can be put in the form

$$-(dT/dx)_i = D_i \, T^{1/2} \tag{35}$$

The upper limit for Equation 35 is called T_b. The value of T_b is found by equating Equations 27 and 20 and solving for T. For the present investigation T_b was found to be sufficiently large that Equation 35 was used for all primary knock-on energies above the ionization threshold E_i.

The ratio R of energy lost in inelastic collisions to energy lost in elastic collisions may be expressed as a function of the primary knock-on energy T. In the intermediate range when $E_i \leq T \leq T_a$, R is proportional to $T^{1/2}$. When $T_a \leq T \leq T_b$, R is proportional to $T^{1/2}/T^{-\alpha}$. Therefore in the intermediate energy range R is always proportional to some power of T and may be generally represented as

$$R = k\,T^{\gamma} \tag{36}$$

where γ is not necessarily an integer and k is a constant independent of energy.

From Equation 31 and Equation 36 the general form for the expression giving the fraction of energy lost due to elastic collisions will be

$$f(T) = \frac{1}{1 + kT^{\gamma}} \tag{37}$$

When $E_i \leq T \leq T_a$,

$$k = D_i/D_c \tag{38a}$$

$$\gamma = 1/2 \tag{38b}$$

The constants D_c and D_i are from Equations 34 and 35.

When $T_a \leq T \leq T_b$,

$$k = D_i/C_c \tag{39a}$$

$$\gamma = 1/2 + \alpha \tag{39b}$$

where C_c and α are from Equation 19.

High energy range

The higher the energy of the primary knock-on the higher the ratio R of energy lost in inelastic collisions to energy lost in elastic collisions. When $R \gg 1$ the fraction f(T) of energy lost due to elastic collisions is approximately

$$f(T) \approx 1/R = T^{-\frac{1}{2}}/k \qquad (40)$$

Energy G(T) Lost in Elastic Collisions

The part of the primary knock-on energy that is dissipated in elastic collisions is found by integrating the fraction f(T) over the entire energy range. Equation 7 illustrates this procedure.

Low energy range

When $T \leq E_i$ the value of f(T) is unity so G(T) = T in this range.

Intermediate energy range

When $E_i \leq T \leq T_a$ the value of G(T) is given by

$$G(T) = E_i + \int_{E_i}^{T} \frac{dT}{1 + k\,T^{1/2}} \qquad (41)$$

where k is given by Equation 38a. Equation 41 is integrated to give

$$G(T) = E_i + \frac{2}{k^2}\Big[k\,T^{1/2} - \ln(1 + k\,T^{1/2}) - k\,E_i^{1/2} + \ln(1 + k\,E_i^{1/2})\Big] \qquad (42)$$

When $T > T_a$ the value of G(T) is given by the general form

$$G(T) = E_i + G(E_i, T_a) + \int_{T_a}^{T} \frac{dT}{1 + kT^{\gamma}} \qquad (43)$$

where $E_i + G(E_i, T_a)$ is given by Equation 42 when $T = T_a$. The term $G(E_i, T_a)$ represents the energy lost in elastic collisions by a particle slowing from energy T_a to E_i.

Unfortunately the exponent γ is not necessarily an integer and the integral

$$G(T_a, T) = \int_{T_a}^{T} \frac{dT}{1 + kT^{\gamma}} \qquad (44)$$

cannot be evaluated directly. Numerical integration was used to obtain a value for $G(T_a, T)$, and hence G(T), from Equation 43.

The method of numerical integration employed the trapezoidal rule. The use of this rule implies that the curve is approximated by straight lines, and the integral is found by taking the area under the set of trapezoids that make up the curve. This can be expressed mathematically by the following expression:

$$\int_{E_i}^{T} f(T)\,dT \approx \left[\Delta_1 T \frac{f(E_i) + f(T_1)}{2} + \ldots + \Delta_n T \frac{f(T_{n-1}) + f(T_n)}{2} \right] \qquad (45)$$

The number n is the total number of intervals taken and $\Delta_n T$ is the energy difference between T_n and T_{n-1}. The fraction of energy lost in elastic collisions at energy T_n is denoted above as $f(T_n)$.

High energy range

When the energy T of the primary knock-on becomes sufficiently high the far greater part of that energy is dissipated in inelastic collisions. Under this condition, $R \gg 1$ and f(T) is given by Equation 40. The energy lost in this range in elastic collisions is thus given by

$$G(T_c, T) = \int_{T_c}^{T} (T^{-\gamma}/k)\,dT = \frac{1}{k(1-\gamma)}\left[T^{(1-\gamma)} - T_c^{(1-\gamma)}\right] \qquad (46)$$

where T_c is that energy where $(dT/dx)_i \gg (dT/dx)_c$ and thus Equation 40 holds. The energy T_c was taken as that value of T for which f(T) = 0.02, i.e., $R = 5_1$, giving in error of less than 2%.

The total expression for G(T) in the high energy range depends upon the value of T_c with respect to T_a. The value of T_c was found to vary from element to element but T_c was always greater than T_a. For the case where $T_a < T_c < T$

$$G(T) = E_i + G(E_i, T_a) + G(T_a, T_c) + G(T_c, T) \qquad (47)$$

The terms $G(T_a, T_c)$ and $G(E_i, T_a)$ have the same form as in Equation 44 and must be evaluated numerically.

Equation 46 was used only for Be and C, the lightest elements investigated. For all other elements the value of T_c was corresponded to a neutron energy greater than 10 Mev. and was thus out of the energy range of interest.

Average Energy $\overline{G(E)}$ Dissipated in Elastic Collisions

Since the initial incident particles are neutrons of energy E, the average energy $\overline{G(E)}$ lost by the primary knock-on in elastic collisions is given in terms of the neutron energy. The general expression used was that of Equation 9. Since different equations hold in different energy ranges the integration had to be broken up and the appropriate expression for G(T) in that energy range used.

Low energy range

When $T \leq E_i$ the primary knock-on loses all its energy in elastic collisions and the average energy lost due to elastic collisions is

$$\overline{G(E)} = T_m/2 = \frac{2A}{(1 + A)^2} E \qquad (48)$$

where A is the atomic number of the stopping material.

Intermediate energy range

For the energy range $E_i \leq T \leq T_a$ the value of $\overline{G(E)}$ was found by integrating Equation 42 over the entire range of knock-on energy and dividing by T_m as given by Equation 8. The expression for $\overline{G(E)}$ in this energy range was then found to be

$$\overline{G(E)} = \frac{1}{T_m} \int_0^{E_i} T\, dT + \frac{1}{T_m} \int_{E_i}^{T_{m(E)}} \left[E_i + G(E_i, T) \right] dT \qquad (49a)$$

$$\overline{G(E)} = \frac{E_i^2}{2T_m} + \left[\frac{2}{T_m k^2} \left\{ \frac{2}{3} kT^{3/2} - \frac{(k^2T-1)}{k^2} \ln(1+kT^{1/2}) - \frac{T^{1/2}}{K} + \frac{T}{2} - HT \right\} + \frac{E_i T}{T_m} \right]_{E_i}^{T_m} \quad (49b)$$

where $H = kE_i^{1/2} - \ln(1 + kE_i^{1/2})$.

When $T_a \leq T \leq T_c$ the average energy lost in elastic collisions was found by numerical integration. The contribution to $\overline{G(E)}$ from energy range $T_a \leq T \leq T_c$ is thus found by using the trapezoidal rule for integrating with respect to T, $G(T_a, T)$ of Equation 44.

<u>High energy range</u>

When $(dT/dx)_i \gg (dT/dx)_c$ the average energy lost in elastic collisions by the primary knock-ons was taken as

$$\overline{G(E)} = (T_c/T_m)\overline{G(T_c)} + (1/T_m) \int_{T_c}^{T_m} \left[G(T_c) + G(T_c, T) \right] dT \quad (50)$$

where $\overline{G(T_c)}$ is the value of $\overline{G(E)}$ where the maximum energy transfer from the neutron to the primary knock-on is T_c. The energy lost due to elastic collisions by a particle while its energy is in the range $T_c \leq T \leq T_m$ is $G(T_c, T_m)$, and is given by Equation 46.

Integrating Equation 50 gives

$$\overline{G(E)} = (T_c/T_m)\overline{G(T_c)} + G(T_c)(T_m - T_c)/T_m$$

$$+ \frac{1}{k(1-\gamma)(2-\gamma)}\left[T_m^{\ 1-\gamma} - (2-\gamma)T_c^{\ 1-\gamma} + \frac{T_c^{2-\gamma}}{T_m}(1-\gamma)\right] \quad (51)$$

Equation 51 was used only for the light elements carbon and beryllium in this study. For the heavier elements $T_m < T_c$ for $E \leq 10$ Mev.

RESULTS

The average energy lost in elastic collisions for the elements investigated is given for various neutron energies up to 10 Mev in Table 1. No values of $\overline{G(E)}$ for neutron energies below 10 kev are listed because all of the primary knock-on kinetic energy is dissipated in elastic collisions below 10 kev for all these elements.

It was found that for the elements investigated the average energy lost due to elastic collisions could be represented by an equation of the form

$$\overline{G(E)} = \frac{E}{Q_1 + Q_2(E-Q_3)^x} \qquad (52)$$

where E is the neutron energy and Q_1, Q_2, Q_3 and the exponent x are constants that are different for each element. These constants were determined graphically from the calculated values for $\overline{G(E)}$ at various energies. The constants Q_1, Q_2, Q_3 and the exponent x determined for each element are given in Table 2.

The constant Q_1 is the ratio of the neutron energy to the average neutron-atom energy transfer $\frac{T_m}{2}$ given by Equation 8; therefore

$$Q_1 = \frac{2E}{T_m} = \frac{(1+A)^2}{2A} E \qquad (53)$$

where A is the atomic number of the target element.

The constant Q_3 in the $(E-Q_3)$ term is the neutron energy corresponding to a maximum energy transfer of E_i, i.e., when $E < Q_2$ there can be no

Table 1. Average primary knock-on energy* lost in elastic collisions

Neutron energy* E	Be	C	Al	Si	Fe	Cu
10	1.80	1.42	0.690	0.670	0.346	0.305
20	3.00	2.84	1.38	1.34	0.692	0.610
40	7.20	5.68	2.76	2.68	1.38	1.22
60	10.2	9.52	4.14	4.02	2.07	1.82
80	12.0	11.5	5.52	5.36	2.76	2.44
10^2	14.2	13.3	6.9	6.70	3.46	3.05
$2x10^2$	21.0	22.5	13.8	13.4	6.92	6.10
$4x10^2$	28.3	34.0	26.1	25.5	13.8	12.2
$6x10^2$	32.9	41.8	35.7	34.9	20.7	18.2
$8x10^2$	36.1	48.3	44.1	42.6	27.6	24.4
10^3	37.9	52.6	51.5	51.3	34.6	30.8
$2x10^3$	39.2	56.8	83.7	85.0	59.3	58.4
$4x10^3$	41.7	64.9	134	145	111.2	108
$6x10^3$	43.3	70.1	178	195	156	150
$8x10^3$	44.3	73.8	215	237	197	195
10^4	45.1	76.2	244	272	237	230

*All energies in kev

Table 2. Emperical constants for Equation 53

Element	Q_1	Q_2	Q_3 (kev)	X
B_e	5.56	2.00×10^{-2}	41.2	1.01
C	7.04	1.20×10^{-2}	71.5	1.01
Al	14.5	6.18×10^{-2}	279	0.660
Si	14.9	7.22×10^{-2}	237	0.631
Fe	28.9	6.82×10^{-2}	1041	0.600
Cu	32.5	5.68×10^{-2}	839	0.55

inelastic collisions. In terms of Q_1, Q_3 may be expressed as

$$Q_3 = \frac{Q_1 E_i}{2} \tag{54}$$

Equation 52 is to be used only when $E > Q_3$. For neutron energies below Q_3 the primary knock-on loses all its energy in elastic collisions. When $E < Q_3$ $\overline{G(E)}$ is the value given by Equation 52 with the $(E-Q_3)$ term set equal to zero.

Expressions for the constant Q_2 and the exponent x were found as functions of the atomic number of the stopping material. These equations are

$$Q_2 = 2.23 \times 10^{-3} \, Z \tag{55}$$

$$x = 1.775 \, Z^{-1/3} \tag{56}$$

All energies in the empirical equations must be expressed in kev.

The equation for average energy lost in elastic collisions by primary knock-ons can be approximated as

$$\overline{G(E)} = \frac{E}{Q_1 + 0.0223\left(E - \frac{Q_1 E_i}{2}\right)^{1.775/Z^{1/3}}} \quad (57)$$

with Q_1 given by Equation 53.

The values given by Equation 57 are shown graphically in Figures 1 through 6. These graphs also show the calculated points from Table 1 and the values obtained by assuming that no elastic collisions occur for knock-on energy T greater than the threshold energy E_i.

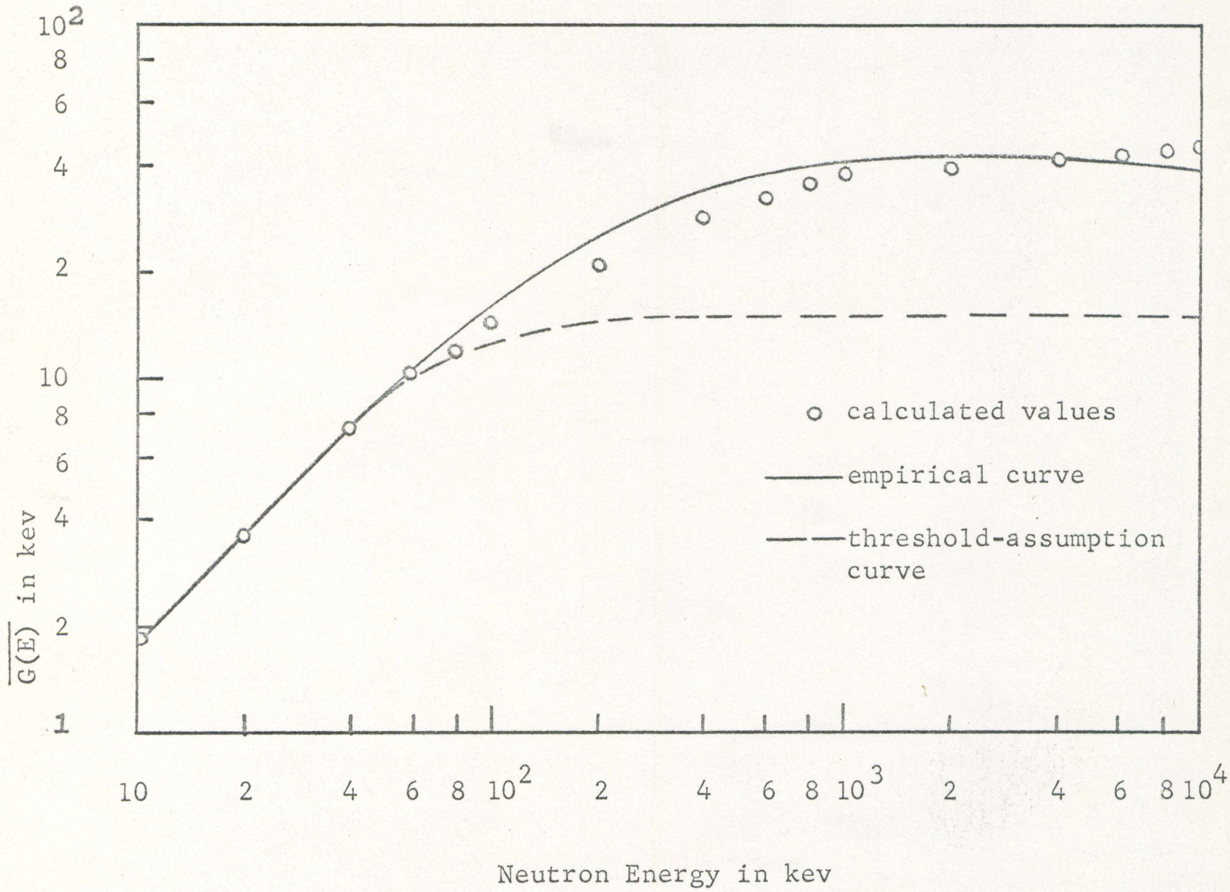

Figure 1. Average energy lost in elastic collisions by primary knock-ons in beryllium

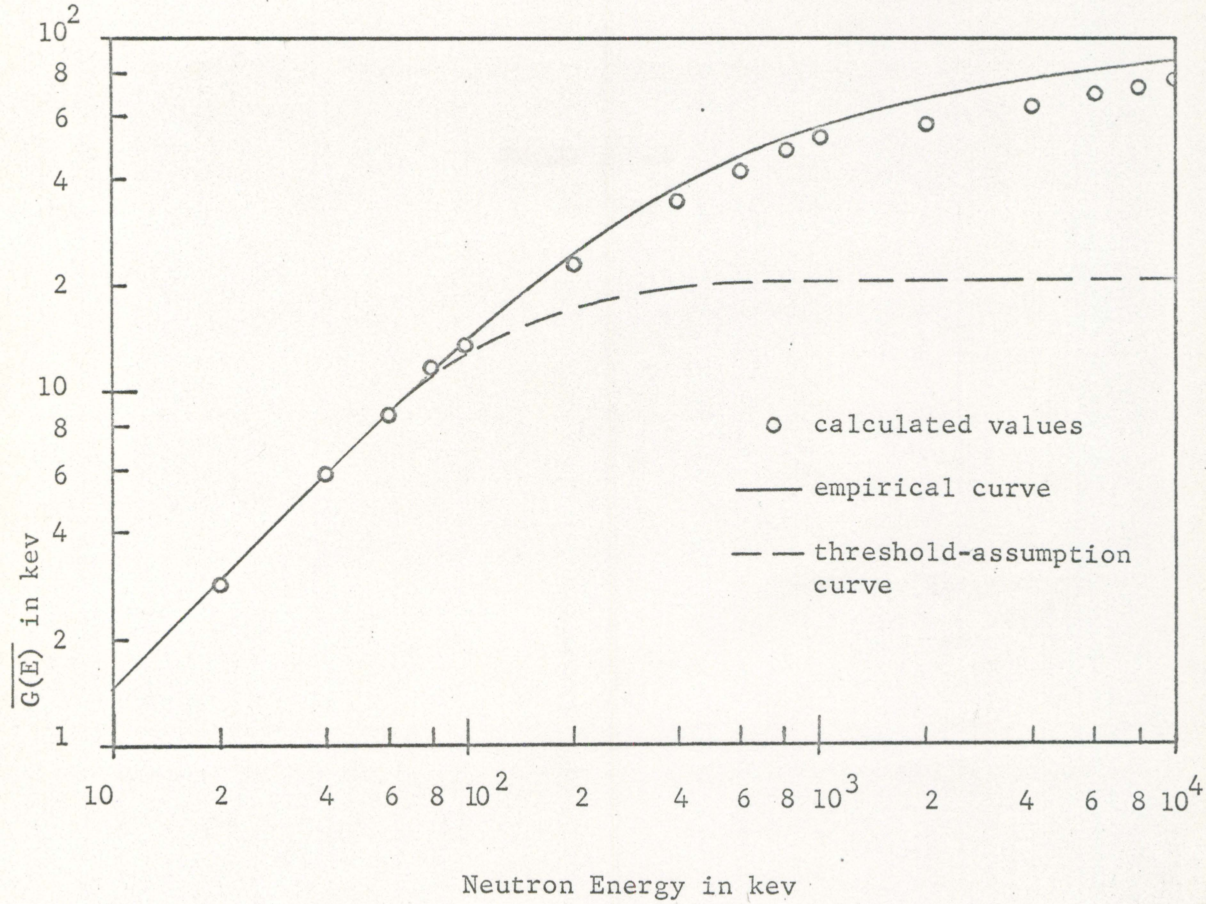

Figure 2. Average energy lost in elastic collisions by primary knock-ons in carbon

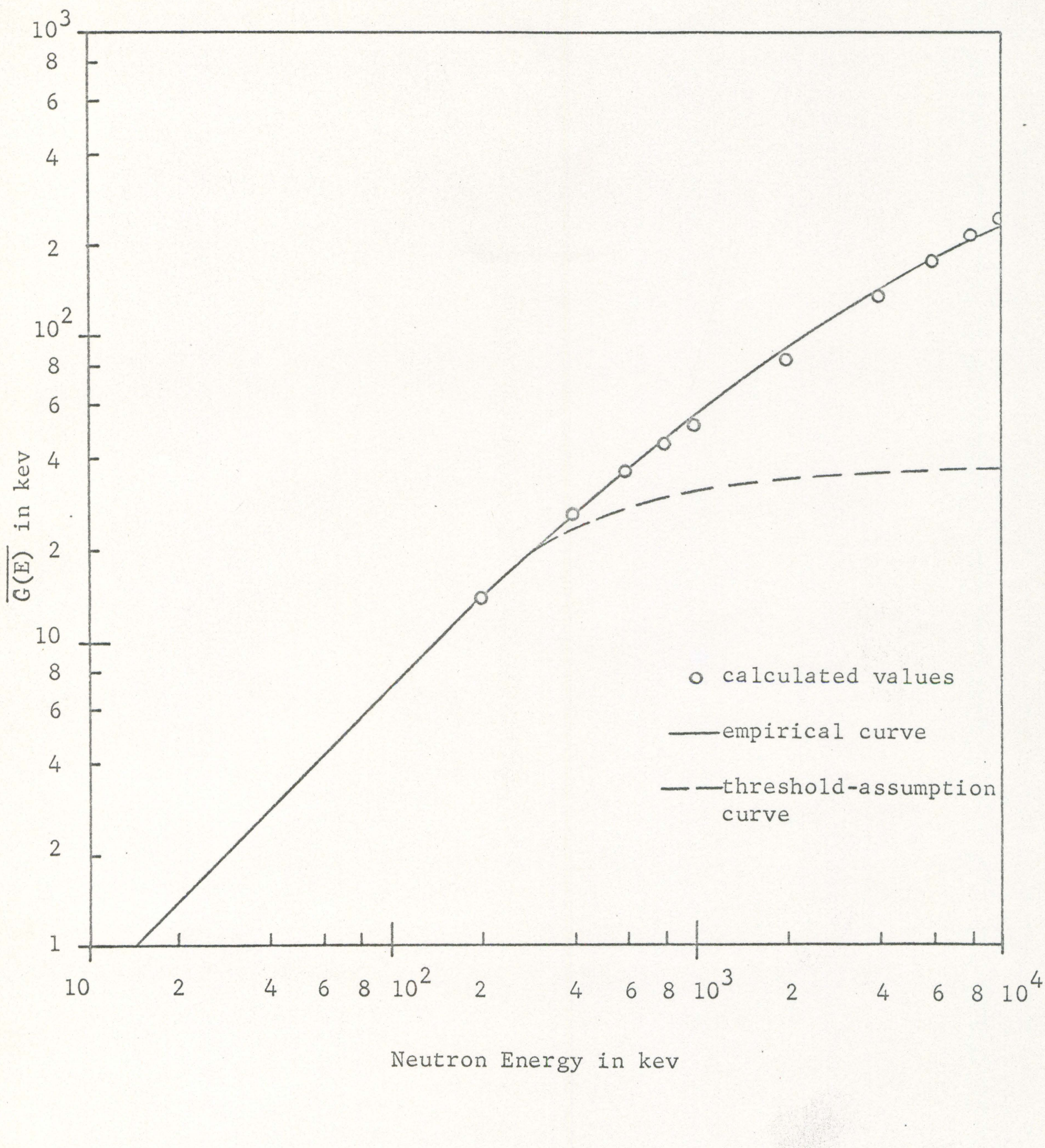

Figure 3. Average energy lost in elastic collisions by primary knock-ons in aluminum

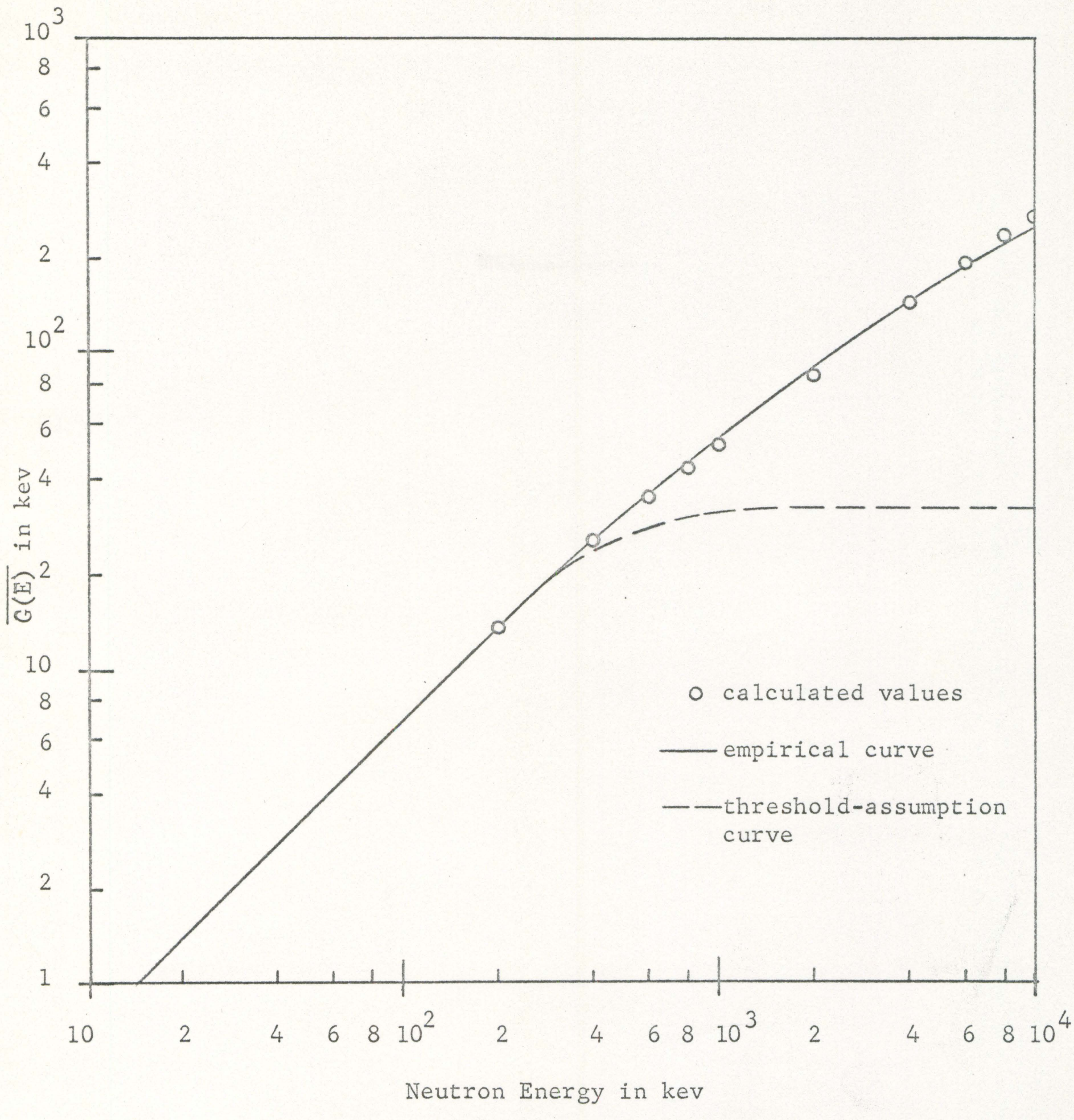

Figure 4. Average energy lost in elastic collisions by primary knock-ons in silicon

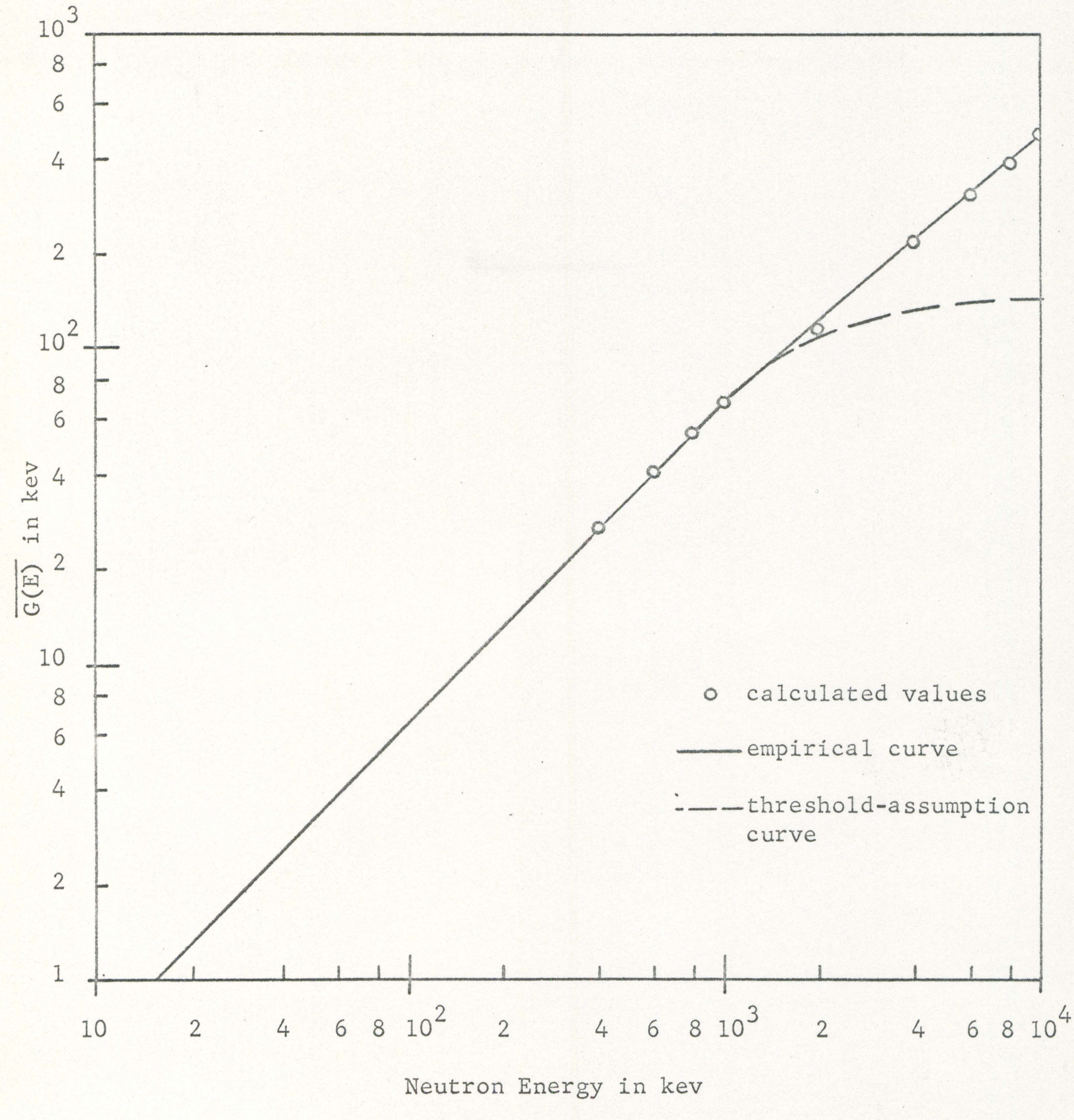

Figure 5. Average energy lost in elastic collisions by primary knock-ons in iron

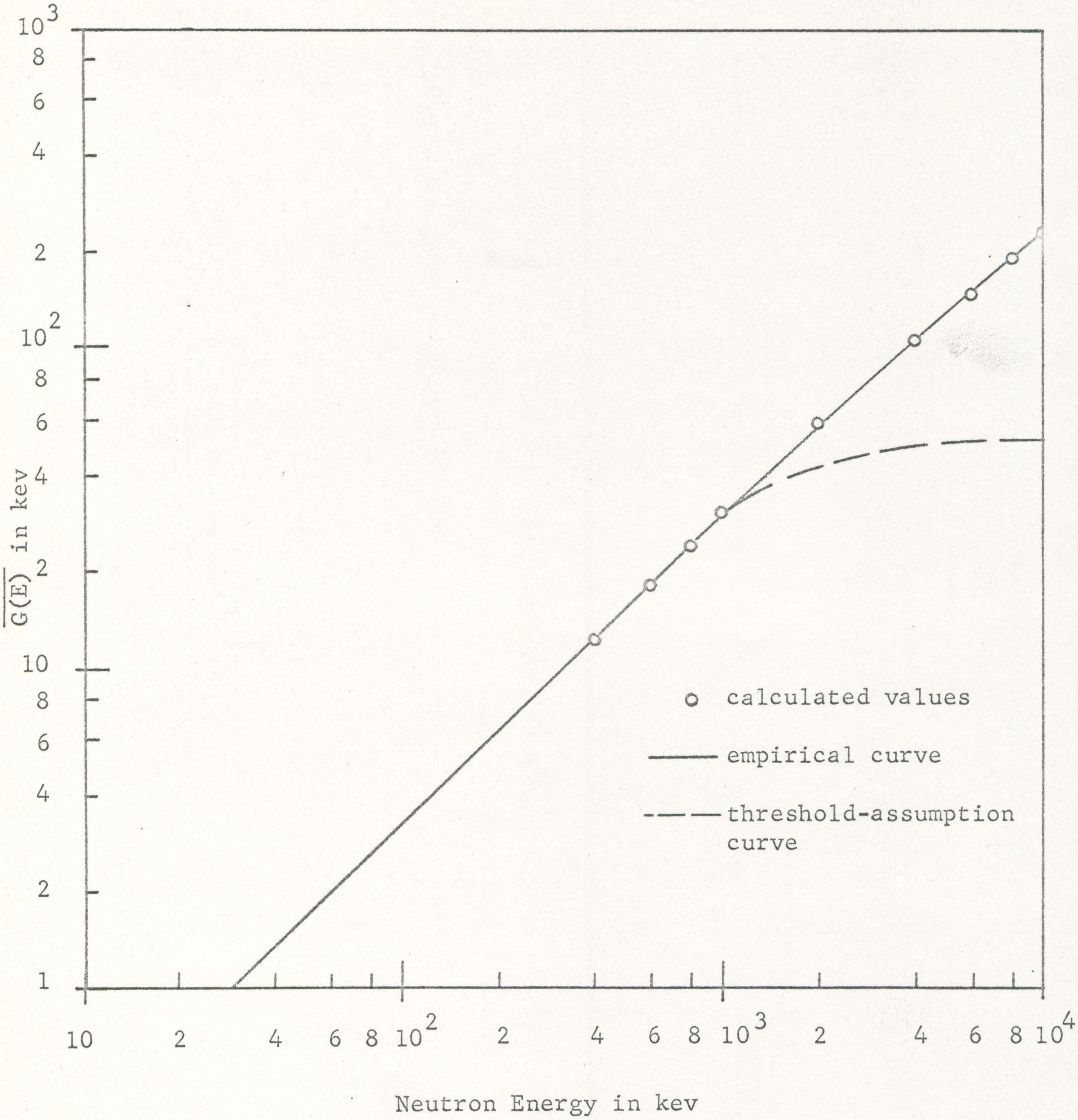

Figure 6. Average energy lost in elastic collisions by primary knock-ons in copper

DISCUSSION

The curves of $\overline{G(E)}$ in Figures 1 through 6 show that the suggested empirical Equation 57 does not give a perfect fit to the calculated points. The greatest difference between the curve and the points is about 15% in the beryllium curve. This disagreement is small enough, however, to warrent the use of the empirical relationship for $\overline{G(E)}$ for nearly all displacement calculations.

Equation 57 does give a much more precise value for the average energy lost in elastic collisions than that value obtained by the usual method of assuming a cut-off energy for elastic encounters. The dotted curves of Figures 1 through 6 indicate the values of $\overline{G(E)}$ given by the "threshold method." The calculated points are as much as eight times greater than the dotted line values. This great difference indicates that the use of the threshold assumption leads to a large underestimation of the energy lost in elastic collisions.

The threshold-assumption values were found from the equation for the energy G(T) lost by a primary knock-on of energy T as given by Snyder and Neufeld (26) and described by Equations 5a and 5b. This theory assumes that all the knock-on energy is lost in elastic collisions when $T < E_i$ and none of this energy is lost in elastic collisions when $T > E_i$. The equation for G(T) was averaged over the entire primary knock-on energy spectrum in the manner of Equation 9. This averaging gave the equation

$$\overline{G(E)} = E_i - (E_i^2/2T_m) \qquad (58)$$

Table 3 compares the results obtained by several methods. The values of Hurwitz and Clark were quoted by Dienes and Vineyard (Table 2.2, 12). The method they used to calculate $\overline{G(E)}$ was essentially the same as that used for the calculated values here. The discrepancy between the values of $\overline{G(E)}$ obtained here and those found by Hurwitz and Clark lies in the fact that different equations for (dT/dx) were used. Because of the inapplicability of the equations used by Hurwitz and Clark, as pointed out in the Review of Literature, the results obtained here should be the more accurate of the two calculations. The values of $\overline{G(E)}$ given for iron are essentially the same for all four cases because the maximum energy transferred by the 1 Mev neutron to a stationary iron atom will not exceed E_i and hence the value of $\overline{G(E)}$ is the average primary knock-on energy $T_m/2$.

Table 3. Comparison of the values of energy* lost in elastic collisions by primary knock-ons resulting from 1-Mev neutrons

	Be	C	Fe
Calculated values	37.9	52.6	34.6
Hurwitz and Clark's values	22	45	34.5
Assumption of sharp threshold	14.7	20.1	34.6
Empirical relation	39.7	56.2	34.6

*All energies in kev

The empirical Equation 57 appears to be reasonable when the limiting cases are considered. As the energy E decreases and approaches the threshold energy $Q_i E_i$ the value of $\overline{G(E)}$ approaches the average primary knock-on energy $T_m/2$, meaning that the change to no inelastic collisions is gradual rather than abrupt. For high neutron energies the loss of energy in elastic collisions becomes proportional to the neutron energy E to the (1-x) power, indicating a slow rise of $\overline{G(E)}$ with increasing E. This high energy proportionality is reasonable because it means that although the percentage of the total energy that goes into elastic collisions decreases, the amount of energy going into elastic collisions still increases with increasing neutron energy.

The main use for Equation 57 is in determining the number of displacements produced in a solid by neutron irradiation. To find the total number of displacements caused by elastic collisions of stationary atoms with both neutrons and primary knock-ons the number of displacements n_d per primary knock-on must be found. Dienes and Vineyard (12) suggest that if the average energy lost by the primary knock-on is known the best estimation for the number of displacements formed per primary knock on is

$$n_d = \overline{G(E)}/2E_d \qquad (59)$$

where E_d is the energy that must be transferred to the stationary atom to displace it. The value of E_d is usually taken to be about 25 ev for all elements.

Comparison of the results obtained here with the experimental data would not be expected to be very meaningful because of the general disagreement between experimental and theoretical displacement values. The experimentally suggested number of displacements formed in a solid is usually less than the number determined theoretically by a factor of 2 or 3 (3, 11). The use of the values of $\overline{G(E)}$ determined here would seem to increase the number of theoretical displacements and make the discrepancy greater.

Despite the apparent disagreement with experimental results as presently interpreted, the use of $\overline{G(E)}$ determined here must be expected to give more accuracy to the theoretical estimation of the number of displacements formed. A large part of the energy that goes into forming displacements, i.e., the energy lost in elastic collisions, is neglected under present-day theory. When this neglected energy is taken into account, as was done here, theoretical pictures become more accurate. The use of the suggested empirical Equation 37, therefore, gives much better estimations of the average energy lost in elastic collisions by primary knock-ons than the previously accepted threshold-assumption method.

LITERATURE CITED

1. Allison, S. K. and Warshaw, S. D. Passage of heavy particles through matter. Reviews of Modern Physics. 25:779-817. 1953.

2. Arnot, F. L. Collision processes in gases. New York, N. Y., John Wiley and Sons, Inc. 1950.

3. Balarin, M. and Hauser, O. The production of radiation effects considered from the point of view of energy relations. (Translated title) Kernenerie 3:973-978. 1960. Original not available; translated in U. S. Atomic Energy Report NP-tr-861. (Technical Information Service Extension, A.E.C.). 1961.

4. Bethe, H. A. and Ashkin, J. Passage of radiations through matter. In Segrè, E., ed. Experimental nuclear physics. Vol. 1. pp. 166-350. New York, N. Y., John Wiley and Sons, Inc. 1953.

5. Bohr, Niels. The penetration of atomic particles through matter. Danske videnskabernes selskab, Copenhagen. Matematiskfysiske skrifter. Medd. 18, No. 8. 1948.

6. Brinkman, John A. On the nature of radiation damage in solids. Journal of Applied Physics. 25:961-970. 1954.

7. Brooks, H. Nuclear radiation effects in solids. Annual Reviews of Nuclear Science. 6:215-276. 1956.

8. Brown, E. and Goldecke, G. H. Effect of atomic interaction potential on defect production in metals. Journal of Applied Physics. 31:932-934. 1960.

9. Bruch, C. A., McHugh, W. E., and Hockenbury, R. W. Variation in radiation damage to metals. Journal of Metals. 8:1362-1372. 1956.

10. Burton, Milton, Radiation chemistry. Journal of Physics and Colloid Chemistry. 51:611-625. 1947.

11. Dienes, G. J. Defects in solids and current concepts of radiation effects. In Harwood, J. J., Hausner, Henry H., Morse, J. G. and Rauch, W. G. The effects of radiation on materials. pp. 1-47. New York, N. Y. 1958.

12. Dienes, G. J. and Vineyard, G. H. Radiation effects in solids. New York, N. Y., Interscience Publishers, Inc. 1957.

13. Francis, Gorden. Ionization Phenomena in Gases. New York, N. Y. Academic Press, Inc. 1960.

14. Holmes, D. K. Theory of radiation damage. U. S. Atomic Energy Commission Report CF-50-7-5 (Oak Ridge National Lab., Tenn.). 1950.

15. Kennard, Earle H. Kinetic theory of gases. New York, N. Y., McGraw-Hill Book Co., Inc. 1938.

16. Kinchin, G. H. and Pease, R. S. The displacement of atoms in solids by radiation. Reports on Progress in Physics. 18:1-51. 1955.

17. Leachman, R B. and Atterling, H. Nuclear collision stopping of astitine atoms. Arkiv för Fysik. 13:101-108. 1958.

18. Lindhard, J. and Scharff, M. Energy dissipation by ions in the kev region. Physical Reviews. 124:128-130. 1961.

19. Lindhard, J. and Scharff, M. Energy loss in matter by fast particles of low charge. Danske videnskabernes selskab, Copenhagen. Matematisk-fysiske skrifter. Medd. 27, No. 15. 1953.

20. Livingston, M. Stanley and Bethe, H. A. Nuclear physics. Pt. C: Nuclear dynamics, experimental. Reviews of Modern Physics. 9:245-390.

21. Rossin, A. D. Radiation damage in steel: considerations involving the effect of neutron spectra. Nuclear Science and Engineering. 9:137-147. 1961.

22. Seitz, Frederick. The effects of irradiation on metals. Science. 138:563-571. 1962.

23. Seitz, Frederick. The modern theory of solids. New York, N. Y. McGraw-Hill Book Company, Inc. 1940.

24. Seitz, Frederick. On the disordering of solids by action of fast massive particles. Discussions Faraday Society. 5:271-282. 1949

25. Seitz, Frederick and Koehler, J. S. Displacement of atoms during irradiation. Solid state physics. 2:305-448.

26. Snyder, W. S. and Neufeld, J. Disordering of solids by neutron radiation. Physical Reviews. 97:1636-1646. 1955.

27. Vaughan, Edward. Stopping power and ion density. U. S. Atomic Energy Commission Report UCRL-2287 (California University, Berkeley, Radiation Lab.). 1953.

ACKNOWLEDGMENTS

The author would like to express his gratitude to Dr. Abdul R. Rana, Professor of Nuclear Engineering, for his advice, guidance, and encouragement given during this investigation.

Also the author would like to thank Dr. Glenn Murphy, Head of the Nuclear Engineering Department of Iowa State University, for departmental supervision.

The author would also like to extend his appreciation to Professor Edward H. Ohlsen, Acting Head of the Engineering Mechanics Department of Iowa State University, for the opportunity to teach in the Engineering Mechanics Department which was a rewarding experience in itself and also enabled the author to receive his education in Nuclear Engineering at Iowa State University.