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Computed effect of neutron irradiation on the concentration of interstitials and vacancies in niobium

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COMPUTED EFFECT OF NEUTRON IRRADIATION ON THE CONCENTRATION OF INTERSTITIALS AND VACANCIES IN NIOBIUM

by

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TABLE OF CONTENTS

I. INTRODUCTION

Extensive effort has been expended in the past to determine the effects of radiation on the physical properties of materials used in reactor construction. This work was started in the early 1940's when Wigner suggested that radiation from an operating reactor may adversely affect material properties. This type of work was then labelled radiation damage research, although all effects of radiation on materials are not necessarily damaging effects. For instance, it has been shown in numerous experimental works that exposure to a sufficiently large integrated flux of fast neutrons will increase the strength of metals. On the other hand, such exposure decreases the ductility of metals. If a strong, non-brittle metal is specified for use, then we have, respectively, a desirable effect and a damaging effect of radiation on the metal. This study will refer to "radiation effects" as opposed to "radiation damage" to prevent the implication that radiation is harmful to materials in all respects. However, the term "radiation defects" will be used to denote crystal structure irregularities resulting from exposure to radiation.

Numerous studies, both theoretical and experimental, have been conducted in the past twenty years in this field. Foremost are the theoretical works of Billington, Brooks, Crawford, Dienes, Kinchin, Koehler, Pease, Seitz, Vineyard, and others who have tendered their own theories or have expanded on existing theories. These theories have attempted to predict the concentration and types of defects in materials caused by prolonged exposure to various kinds of radiation. With these predictions

at hand, attempts have been made to explain how the defects will affect some of the physical properties of materials.

On the other hand, many researchers have experimentally determined radiation effects in materials without attempting to explain the observed results of their studies in theoretical terms. Inasmuch as this approach was necessary for the rapid growth in the number of nuclear installations up to the present time, the point has been reached where it is advantageous to explain with greater precision the effects of radiation on materials and not merely to state observed experimental results.

Researchers are concerned with radiation effects in several different types of reactor construction materials, among them metals, semiconductors, plastics, ceramics, and graphite. Radiation may affect each of these materials differently. This study will deal with radiation effects in metals, generally, and with radiation effects in niobium, specifically.

Neutrons, charged particles, fission fragments, and electromagnetic radiation may each affect metals in different ways. An atomic transmutation effect resulting from neutron capture and subsequent radioactive decay is also present. However, a large part of the permanent radiation effects observed in metals in a reactor (with the exception of fission-fragment effects in the fuel elements) is due to the interaction of fast neutrons with the metal atoms. This study will be concerned with the permanent effects of fast neutron interaction with metals, neglecting all other effects despite their possible importance.

Attempts have been made to correlate theoretical and experimental

estimates of defect concentrations caused by fast neutrons using the change in electrical resistivity of an irradiated sample. It has been found that in many cases defect concentrations readily anneal out at temperatures considerably lower than room temperature. Experiments have been performed at temperatures approaching absolute zero to minimize temperature effects on the annealing of radiation defects. Using the best techniques now at hand, theoretical estimates of defect concentrations are often ten to twenty times in excess of the number estimated in experimental checks on theory. This discrepancy may be due to excessive annealing of the defects, or it may be due to inaccuracies in the theory used to interpret the experimental results.

Even though estimates have been made of defect concentrations, it has been impossible up to now to predict accurately a theoretical relationship between defect concentrations and changes in the macroscopic properties of metals. However, many experiments have been performed to determine the relationship between integrated neutron flux and changes in macroscopic properties of interest. Often these are of little value because of the failure to report the neutron energy spectrum, since the radiation effect produced by a fast neutron is dependent in a complex way on its energy. If some way could be devised to portray accurately the relationship between the true neutron flux (energy dependent) and the resulting defect concentrations, then the relationship between changes in defect concentrations and changes in macroscopic properties of interest could be more accurately determined.

A defect in a metal is an irregularity in the lattice pattern.

Basically, defects are of two types (neglecting foreign atoms)--vacancies and interstitial atoms. They are produced when a neutron collides with an atom (directly or indirectly) to remove it from its regular lattice position, resulting in the production of a vacancy and an interstitial. Either type of defect may migrate to a sink and be annihilated. Vacancies and interstitials are thought to migrate at different rates, and thus, at any given time, there may be more of one type of defect than the other. An interstitial may recombine with a vacancy during migration to cause annihilation of the pair. Vacancies or interstitials may also combine in various ways to produce more complex types of defects such as defect clusters or dislocations.

This study is a theoretical exposition of the relationship between neutron flux (energy dependent) and the formation and extermination of defects in niobium metal. A mathematical model is developed showing this relationship in terms of geometry, time, neutron energy and density, and other variables which are described later on.

II. OBJECTIVE

The objective of this dissertation is to develop (on a macroscopic scale) equations describing the production and annealing of interstitial atoms and vacant lattice sites in niobium metal which is in the presence of a steady-state neutron flux. The equations developed in this work are solved for the purpose of illustration (using assumed representative values where necessary). A method is devised which allows one to describe the steady-state neutron flux arising from an infinite plane source of neutrons with a certain spectrum of energies. The neutron flux is thus energy dependent. This flux is used in the solutions of the equations.

The general form of the equations in this work was suggested by Aqua and Allio (3), but they did not attempt to develop the equations. To their equations was added a term to account for the radiation-induced annealing which takes place as a result of localized thermal-spike heating.

III. LITERATURE REVIEW

Work on radiation effects in materials has progressed rapidly in the past ten years. This increased activity has arisen because of the use or proposed use of high-powered nuclear reactors operating for long periods of time. Thus, radiation effects on materials assumes an important role in the nuclear reactor field. There is a large amount of information available on past and present radiation effects work, both experimental and theoretical.

The Radiation Effects Information Center of Battelle Memorial Institute issues periodic reports in the field. The Center attempts to keep abreast of all developments in the field, both experimental and theoretical.

The work by Billington and Crawford (10) is a general, theoretical exposition of radiation effects, starting with elementary ideas and building up to a complex discussion of the field. The work of Dienes and Vineyard (29) is similar, but is not as thorough or complex.

Barnes (4,5) deals with the theory associated with clusters of point defects in irradiated metals. He explains the clusters in terms of irregularities that appear in the crystal structure and gives simple mathematical expressions for defect concentrations.

Blewitt et al. (11) use experimental results dealing with resistivity changes in irradiated metals to support some of their proposed theory. They also discuss various annealing processes associated with radiation defects.

Brinkman (13) examines, on the microscopic or atomic scale, the

radiation effects produced in a metal by knock-on atoms (taking into account the energy of the knock-ons). He discusses the theory of the production of displaced atoms and other lattice imperfections resulting from particle bombardment, the nature and mobility of the imperfections and their role in annealing and recovery, and the relationship between radiation-produced imperfections and observable properties. He believes that a classical description of the collision process is more appropriate than a quantum mechanical description throughout the energy ranges encountered in practice. Brinkman also developed an estimate of the collision radius in the "hard sphere" range of collisions between knock-on atoms, and presented theory which predicts the number of secondary displacements produced by a primary knock-on atom. Uncertainties in his work included the estimate of the "hard sphere" collision radius and the lack of an adequate theory to explain energy loss by electronic excitation and ionization for very slow charged particles.

Many authors contributed articles on radiation effects which appeared in the Proceedings of the International Conference on the Peaceful Uses of Atomic Energy. This conference presented many new ideas in the field and also prompted the declassification of material already developed. A second conference followed two years later to present material not given at the first conference. These two conferences presented papers by many of the leading radiation-effects people throughout the world.

Seitz and Koehler (73-77) are two authorities concerned with the theory of displacement of atoms during irradiation and have produced several works in the field which cover the subject rather thoroughly.

Other works deal mainly with observable macroscopic effects of radiation on materials and, in most cases, do not attempt to explain thoroughly the observable results in theoretical terms.

IV. DISCUSSION OF THE PROBLEM

This dissertation is a theoretical exposition of the relationship between a steady-state neutron flux and the concentration of defects in irradiated niobium.

Niobium metal is chosen for use in the model because it is representative of the body-centered cubic family of metals. Niobium metal is also of interest because of its use or contemplated use as a reactor construction material. However, the choice of material for use in the model is more or less arbitrary, since many of the fundamentals of radiation effects are not dependent upon the properties of any particular isotope or element. Those parts of the development which are dependent upon such specific properties are easily recognizable when encountered.

The physical model consists of an infinite plane source of fission neutrons surrounded by an infinite expanse of niobium metal. The geometrical simplicity of the model prevents unnecessary complications from arising in the neutron flux determination, which is an auxiliary part of the development.

In attempting to determine the radiation effects produced in the niobium, it is found that many variables enter. A listing of these variables may be given in several categories. The variables associated with the neutron flux are the neutron density, the neutron energies, direction of travel of the neutrons, atomic weight of the neutrons, and the cross sections for neutron collision and absorption. Defect variables are the type of defect, minimum energy for defect production, minimum energy for defect migration, and the direction for defect migration.

Variables associated with the niobium metal include its lattice structure and the atomic weight and number of the niobium atoms. Other variables are time, geometry, temperature, and the previous history of the niobium metal.

Some of the variables are inherently fixed. The atomic weights and numbers of the various atoms or particles in question are fixed constants. The lattice structure of niobium is body-centered cubic at all temperatures.

Others of the variables can be arbitrarily fixed. It is assumed that the niobium metal is completely annealed and also free of any radiation effects before exposure to a neutron flux. Complete annealing insures that no cold-working effects are present. (Cold working and exposure to neutron radiation each produce similar effects in metals.) The number of neutrons from the source can be fixed at any convenient value. The temperature of the material is assumed to be constant at 0° C.

Only two types of crystal radiation defects will be considered--interstitial atoms and vacant lattice sites. These two types probably appear in more complex form than single defects, but it is thought that a workable model can be developed using these two defects which will illustrate the principles of radiation effects.

Because of the system selected, the only geometrical variable which will enter the problem is the perpendicular distance from the neutron source, and results will be the same for both negative and positive directions. Time is a major variable.

The remaining variables enter in a more complex manner, and their

influence on the problem is difficult to analyze. The energy of the neutrons from the source is taken to be a typical fission spectrum closely approximated by $S(E) = 0.76985\ E^{\frac{1}{2}} \exp(-0.775E)$, as given by Weinberg and Wigner (97), in which E is the neutron energy in Mev, and S(E) is the number of fission neutrons per unit energy normalized to one fission neutron.

The cross sections for neutron collision and neutron absorption in a particular material are often dependent on the energy of the neutron. This dependence is accurately described by graph in most cases. Values used in this work may be found in Hughes and Schwartz (42).

It will be assumed in this problem that it is equally probable for a neutron to travel in any direction, regardless of circumstances. It is further assumed that source neutrons will be emitted isotropically and scattering will be elastic and spherically symmetric in the laboratory system. A slight error is thereby introduced for high-energy neutrons which will be partly corrected by neglecting the inelastic scattering of neutrons.

The minimum energy for defect production is dependent on the direction in which the atom is displaced. An atom will require greater energy to be displaced directly toward a nearest neighbor than between two atoms. The orientation of the niobium crystals with respect to the oncoming neutron or primary (or secondary, tertiary, etc.) knock-on atom is also a factor entering into the determination of the mimimum energy for defect production. The energy and direction for defect migration are also related in like manner. This complexity will be simplified by using

averaged values for the defect production and migration energies.

A direct approach to the problem of finding the concentration of radiation defects is to determine first the steady-state neutron flux in the niobium as a function of neutron energy and distance from the source. Once this flux is determined, it can be used to determine the concentration of defects produced at any particular point as a function of time. The development beginning in the next section will thus first concern the determination of the steady-state neutron flux in the model.

V. DERIVATION OF EQUATIONS

A. Steady-State Neutron Flux

The equations for the steady-state neutron flux in the model will be rigorously developed using the principles of Placzek (65), Weinberg and Wigner (97), and Glasstone and Edlund (33) for the continuous slowing down of neutrons.

The first item considered in the development will be the slowing down density, $q(E)$, defined as the number of neutrons per cubic centimeter per second that slow down past a given energy. Since the slowing down occurs in a moderator of mass number greater than unity, it is necessary to determine $q(E)$ in several intervals close to the source energy and also for the asymptotic case. However, the development will be carried through assuming that the asymptotic case is valid for all energy ranges. A correction term will then be developed which can be applied to the asymptotic values in the energy ranges near the source energy which will give the true $q(E)$ for all energy ranges. This correction term comes from the work of Placzek (65).

In the asymptotic case it is known that the collision density per unit energy, $F_{as}(E) = \Sigma_s(E)\,\phi_{as}(E)$, is proportional to $1/E$, or $F_{as}(E) = \text{constant}/E$. The slowing down density is given by

$$q(E) = \int_E^{E/\alpha} \Sigma_s(E')\,\phi_{as}(E')\,\frac{E - \alpha E'}{E'(1 - \alpha)}\,dE' , \qquad (1)$$

where the neutron energy, E, lies in the asymptotic range. Σ_s is the

macroscopic scattering cross section, and α is given by

$$\alpha = (A - 1)^2/(A + 1)^2 .$$

In another form, equation 1 becomes

$$q(E) = \int_E^{E/\alpha} F_{as}(E') \frac{E - \alpha E'}{E' (1 - \alpha)} dE' \tag{2a}$$

$$= \int_E^{E/\alpha} (\text{constant}/E') \frac{E - \alpha E'}{E' (1 - \alpha)} dE' \tag{2b}$$

$$= \text{constant } (1 + \frac{\alpha}{1 - \alpha} \ln \alpha) = \zeta \text{ constant}. \tag{2c}$$

First, a solution will be obtained which does not allow for neutron capture. This solution will then be modified to include neutron absorption during the slowing down process. Thus, for all energies, the slowing down density must be constant and equal to the source strength, since all source neutrons must slow down past any given energy greater than thermal energy. Equation 2c now becomes

$$q(E) = \zeta \text{ constant} = \text{source strength}. \tag{3}$$

Therefore,

$$F_{as}(E) = \frac{\text{source strength}}{\zeta E} = \Sigma_s (E) \phi_{as} (E). \tag{4}$$

Since $q(E)$ equals the source strength, it is also true that

$$q(E) = \zeta \Sigma_s (E) E \phi_{as} (E), \tag{5}$$

which is the asymptotic slowing down density without capture.

If there is no absorption of neutrons after a diffusion time t, as is being assumed, then

$$D\, v\, \nabla^2\, n(\underline{r},t) = \frac{\partial\, n(\underline{r},t)}{\partial\, t}\ . \tag{6}$$

The decrease in $\ln E$ due to collisions with moderator nuclei is given by

$$-d \ln E = du = \frac{\zeta\, v}{\lambda_s}\, d\, t, \tag{7}$$

where v is neutron velocity and λ_s is the scattering mean free path. Allowing the lethargy interval, du, to correspond to the time interval, dt, it is found that

$$n(\underline{r},u)\ du = n(\underline{r},t)\ dt\ , \tag{8a}$$

or

$$n(\underline{r},t) = (\zeta v/\lambda_s)\ n(\underline{r},u). \tag{8b}$$

It follows from equations 8a-b that

$$\frac{\partial n(\underline{r},t)}{\partial t} = (\partial u/\partial t)\ \left|\partial n(\underline{r},t)/\partial u\right|$$

$$= (\zeta v/\lambda_s)\ \left|\partial(\zeta v/\lambda_s)(n(\underline{r},u))/\partial u\right|. \tag{9}$$

Therefore,

$$D\, v\, \nabla^2\, n(\underline{r},t) = \partial n(\underline{r},t)/\partial t \tag{6}$$

becomes

$$D\, \nabla^2 \left[\zeta v\, n(\underline{r},u)/\lambda_s\right] = \zeta/\lambda_s \left[\partial(\zeta v/\lambda_s)\left|n(\underline{r},u)\right|/\partial u\right]. \tag{10}$$

Since

$$v\, n(\underline{r},u) = \phi\,(\underline{r},u) \tag{11}$$

and

$$\lambda_s = 1/\Sigma_s\ , \tag{12}$$

equation 10 becomes

$$D\, \nabla^2 \left|\zeta\, \Sigma_s\, \phi(\underline{r},u)\right| = \zeta\, \Sigma_s\, \frac{\partial}{\partial u} \left[\zeta\, \Sigma_s\, \phi(\underline{r},u)\right] \tag{13a}$$

or

$$D\, \nabla^2\, q(\underline{r},u) = \zeta\, \Sigma_s\, \frac{\partial q(\underline{r},u)}{\partial u}\ . \tag{13b}$$

The definition

$$\tau(u) = \int_0^u \frac{D}{\zeta\, \Sigma_s}\, du \tag{14}$$

may be inserted in equation 13b to give

$$\nabla^2\, q(\underline{r},\tau) = \frac{\partial q(\underline{r},\tau)}{\partial \tau}\ . \tag{15}$$

The definition in equation 14 may also be given in terms of energy, in which case

$$\tau(E) = \int_{E}^{E_o} \frac{D}{\zeta \Sigma_s} \cdot \frac{dE}{E} \quad . \tag{16}$$

For an infinite plane source of fast neutrons where the source lies in the y,z-plane, equation 15 becomes

$$\nabla^2 q(x,\tau) = \frac{\partial q(x,\tau)}{\partial \tau} \quad . \tag{17}$$

At the source, the neutron age is zero, and $q(x,0) = S\ \delta(x)$, $\delta(x)$ being the Dirac delta function and S being the fast neutron source strength in neutrons per cubic centimeter per second, all with source energy.

Separate the variables in equation 17 by letting

$$q(x,\tau) = X(x)\ T(\tau) \quad . \tag{18a}$$

Then

$$(1/X)(d^2X/dx^2) = (dT/d\tau)(1/T) \quad . \tag{18b}$$

One side is a function of x only and the other a function of τ only, so both must be equal to a constant, $-\Lambda^2$, where Λ^2 is a real positive quantity. Therefore, the solutions to the two resulting differential equations are

$$X = A' \cos \Lambda x + C' \sin \Lambda x \quad \text{and} \quad T = F \exp(-\Lambda^2) \quad , \tag{19}$$

and the original equation becomes

$$q = \exp(-\Lambda^2 \tau)(A'' \cos \Lambda x + C \sin \Lambda x). \tag{20}$$

With the use of the Fourier integral, it is found that

$$q(x,\tau) = \frac{1}{\pi}\int_0^\infty d\Lambda \int_{-\infty}^{\infty} S\delta(x') \exp(-\Lambda^2\tau) \cos\left[\Lambda(x'-x)\right] dx' \ . \qquad (21)$$

Equation 21 may be integrated with respect to Λ to give

$$q(x,\tau) = \frac{1}{\sqrt{4\pi\tau}}\int_{-\infty}^{\infty} S\delta(x') \exp[-(x'-x)^2/4\tau]dx' \ . \qquad (22)$$

It is known that

$$\int_{-\infty}^{\infty} f(x') \delta(x') dx' = f(0) \ , \qquad (23)$$

so that

$$q(x,\tau) = \frac{Se^{-x^2/4\tau}}{\sqrt{4\pi\tau}} \ . \qquad (24)$$

This expression gives the number of neutrons from an infinite plane source of strength S, per cubic centimeter per second at x, which slow down past a given energy E. This equation can be modified to make it more detailed and more explicit with respect to source neutron energies. The resulting equation is

$$q(x,E_0,\tau) = \frac{S(E_0) \exp\left[-x^2/4\tau(E_0)\right]}{\sqrt{4\pi\tau(E_0)}} \ , \qquad (25)$$

which is the number of neutrons, per cubic centimeter per second at x,

which slow down past a given energy E from a source of strength $S(E_o)$, where E_o is the source neutron energy.

With the use of equation 25, it is seen that

$$\phi(x, E_o, \tau) = \frac{S(E_o)\ \exp\left[-x^2/4\tau(E_o)\right]}{\zeta\ \Sigma_s(E)\sqrt{4\pi\tau(E_o)}} \ , \tag{26}$$

which expression gives the flux per unit lethargy at energy E at position x contributed to solely by source neutrons with energy E_o (assuming no capture).

It will now be assumed that the absorption cross section varies slowly in the energy range considered (10 Mev to thermal). This is approximately true for niobium in all ranges of interest. Thus,

$$q(E) = \int_E^{E/\alpha} F_s(E')\ \frac{E - \alpha E'}{E'(1 - \alpha)}\ dE' \ , \tag{27}$$

where $F_s(E')$ is now the scattering collision density and not the total collision density as given before. Transferring the variable from energy to lethargy ($u = \ln E_o/E$), the equation becomes

$$q(u) = \int_{u+\ln\alpha}^{u} \frac{F_s(u')}{1 - \alpha}\ (e^{u'-u} - \alpha)\ du' \ . \tag{28}$$

It is assumed that $F_s(u)$ varies slowly over a lethargy interval, so that $F_s(u')$ can be closely approximated by the first two terms of a Taylor series expansion about u. Therefore,

$$q(u) = \frac{1}{1-\alpha} \int_{u+\ln\alpha}^{u} \left[F_s(u) + (u' - u) \frac{dF_s(u)}{du} \right] (e^{-u} e^{u'} - \alpha)\, du' \quad (29)$$

$$= \zeta F_s(u) + a \frac{dF_s(u)}{du} \quad , \quad (30)$$

where

$$\zeta = 1 + \frac{\alpha}{1-\alpha} \ln \alpha \quad (31)$$

and

$$a = \frac{\alpha - \alpha\ln\alpha + \frac{1}{2}\alpha (\ln\alpha)^2 - 1}{1-\alpha} \, . \quad (32)$$

Again,

$$q(u) = \int_{u+\ln\alpha}^{u} \frac{F_s(u')}{1-\alpha} (e^{u'-u} - \alpha)\, du' \quad (33)$$

and

$$\frac{dq(u)}{du} = F_s(u) - \frac{1}{1-\alpha} \int_{u+\ln\alpha}^{u} F_s(u')\, e^{u'-u}\, du' \quad (34)$$

$$= F_s(u) - \frac{1}{1-\alpha} \int_{u+\ln\alpha}^{u} \left[F_s(u) + (u'-u) \frac{dF_s(u)}{du} \right] e^{u'-u} du' \, . \quad (35)$$

Equation 35 can be integrated to give

$$dq/du = \zeta\, dF_s(u)/du \, . \quad (36)$$

Multiply equation 30 by ζ and equation 36 by a, and obtain the

difference between the results. In this manner it is found that

$$\zeta\, q(u) - a\, dq(u)/du = \zeta^2\, F_s(u) \ . \tag{37}$$

It is known that $-dq = \Sigma_a\, \phi(u)\, du$, since the decrease in the slowing down density must be equal to the number of neutrons absorbed per cubic centimeter per second in the lethargy interval du. Therefore,

$$dq/du = -\Sigma_a\, \phi(u) \tag{38}$$

may be substituted in equation 37 to give

$$\phi(u) = q(u)/(\zeta\, \Sigma_s + \gamma\Sigma_a) \ , \tag{39a}$$

where

$$\gamma = -a/\zeta \ . \tag{39b}$$

In like manner, it is found that $\tau(u)$, with slowly varying capture, becomes

$$\tau(u) = \int_0^u \frac{D}{\zeta\Sigma_s + \gamma\Sigma_a}\, du \ . \tag{40}$$

Therefore, to make equation 26 valid for slowly varying capture, it must be modified as above to give

$$\phi(x,E_0,\tau) = \frac{S(E_0)\, \exp[-x^2/4\tau(E_0)]}{(\zeta\Sigma_s + \gamma\Sigma_a)\, \sqrt{4\pi\tau(E_0)}} \ , \tag{41}$$

where $\tau(u)$ is given by equation 40.

In review, equation 41 is valid for slowly varying capture assuming

asymptotic slowing down in all energy ranges. To correct for non-asymptotic slowing down where E is near the source energy E_o, the development of Placzek (65) must be used.

The correction factor may be found in the following manner assuming no neutron capture. Let $y = E_o/E$. $K(y)\, dy/y$ represents the average number of collisions which a neutron undergoes in the interval from $\ln y$ to $\ln y + d \ln y$.

Let $p(y,y')\, dy/y$ be the probability that a neutron will lie in the interval dy after one collision if its energy before the collision was E_o/y' (or E'). The probability is unity that the neutron will be somewhere in the interval zero to infinity, or

$$\int_0^\infty p(y,y')\, dy/y = 1 \,. \tag{42}$$

At steady state (with no absorption) the number of collisions in an interval dy/y must be equal to the number of collisions which bring a neutron from the interval dy'/y' into the interval dy/y. This is given by

$$K(y') \left[p(y,y')\, dy/y\right] dy'/y' \tag{43}$$

(or the average number of collisions which a neutron undergoes in the interval from $\ln y'$ to $\ln y' + d \ln y'$ times the probability that such a neutron will lie in the interval dy after the collision).

For steady state, it is evident that

$$K(y)\,dy/y = p(y,1)\,dy/y + \left[\int_0^\infty K(y')p(y,y')dy'/y'\right] dy/y \qquad (44a)$$

or

$$K(y) = p(y,1) + \int_0^\infty K(y')p(y,y')\,dy'/y' \,, \qquad (44b)$$

where $p(y,1)\,dy/y$ is the probability that a source neutron will lie in the interval dy after only one collision. When the moderator atom has mass greater than unity, the neutron energy may go no lower than αE from a collision at E, where

$$\alpha = (A-1)^2/(A+1)^2 \,. \qquad (45)$$

For spherically symmetric scattering, it is equally probable that the neutron energy will lie anywhere in the interval E to αE after scattering. In terms already used, this means that

$$p(y,y') = (1/1 - \alpha)(y'/y) \text{ for } \alpha y < y' < y \qquad (46)$$

$$= 0 \qquad \text{for } y' < \alpha y \text{ and } y' > y. \qquad (47)$$

Since it is not possible for a source neutron to be degraded below αE_o in energy as a result of its first collision, equation 44b must be written for each region above and below αE_o in energy and solved separately in each region. Below αE_o, there is no contribution from first collisions of source neutrons, so equation 44b for this case becomes

$$K(y) = \int_0^\infty K(y')\,p(y,y')\,dy'/y' \,. \qquad (44c)$$

The values for $p(y,y')$ may be inserted in equations 44b-c to give

$$K(y) = \frac{1}{(1-\alpha)\, y} + \frac{1}{(1-\alpha)\, y} \int_1^y K(y')dy' \quad \text{for } 1 \leq y < 1/\alpha \tag{48a}$$

$$= \frac{1}{(1-\alpha)\, y} \int_{\alpha y}^y K(y')\, dy' \qquad \text{for } y > 1/\alpha \ . \tag{48b}$$

Equation 48a can be solved directly by differentiating both sides with respect to y. This gives

$$d\, K(y)/d\, y = \left[K(y)/y\right] (\alpha/1 - \alpha) \ , \tag{49a}$$

or

$$d\, K(y)/K(y) = dy/y\ (\alpha/1 - \alpha) \ . \tag{49b}$$

From equation 49b it follows that

$$K(y) = \text{constant}\ (y^{(\alpha/1-\alpha)}) \ . \tag{50}$$

A boundary condition is that $K(1) = 1/(1 - \alpha)$. Therefore, $1/(1-\alpha) =$ constant, and

$$K(y) = y^{(\alpha/1-\alpha)}/1 - \alpha \ . \tag{51}$$

Let the solution in this first energy range be denoted by $K_o(y)$.

The solution of equation 48b is more complicated. Its solution is initiated by introducing a change of variable as follows:

$$z_n = \frac{\alpha^{\frac{1}{1-\alpha}}}{1-\alpha} \ln \alpha^n y \ , \tag{52}$$

where the solution $K_n(y)$ is valid for the energy range $\alpha^{-n} \leq y \leq \alpha^{-n+1}$. Let

$$K_n(y) = K_0(y)\ J_n(z)\ , \tag{53}$$

where $J_n(z)$ is some function of z.

When equations 52 and 53 are substituted in equation 48b, it is found that

$$J_n(z) = J_n(0) - \int_0^z J_{n-1}(z')\ dz' \quad \text{for} \quad n > 0 \tag{54a}$$

$$= 1 \qquad \text{for} \quad n = 0. \tag{54b}$$

By recurrent application of equations 54a-b, it is found that

$$J_n(z) = \sum_{m=0}^{n} J_{n-m}(0)\ (-z)^m/m!\ . \tag{55}$$

The quantity K is continuous except at $y = 1/\alpha$. Therefore,

$$J_n(0) = J_{n-1}(\theta) \qquad \text{for} \quad n > 1\ , \tag{56}$$

where $\theta = \alpha^{\frac{1}{1-\alpha}} \ln(\alpha^{-\frac{1}{1-\alpha}})$. This is true because z varies between zero and θ in each interval considered, and the value of $J_n(z)$ at the higher-energy end of the lower-energy interval equals the value of $J_{n-1}(z)$ at the lower-energy end of the adjacent higher-energy interval.

It is known that

$$K_1(\alpha^{-1}) = \frac{\alpha}{1-\alpha}\ (\alpha^{-\frac{1}{1-\alpha}} - 1)\ , \tag{57}$$

so that

$$J_1(0) = J_o(\theta) - \alpha^{\frac{1}{1-\alpha}} = 1 - \alpha^{\frac{1}{1-\alpha}} . \tag{58}$$

When equation 56 is substituted in equation 55, it is found that

$$J_{n-1}(\theta) = J_n(0) = \sum_{m=0}^{n-1} J_{n-m-1}(0)(-\theta)^m/m! \quad \text{for } n > 1 . \tag{59}$$

From equations 58 and 59,

$$J_n(0) = A_n(\theta) - \alpha^{\frac{1}{1-\alpha}} A_{n-1}(\theta) , \tag{60}$$

where

$$A_n(\theta) = \sum_{m=0}^{n-1} (m-n)^m \theta^m/m! \tag{61}$$

and

$$A_o(\theta) = 1 \quad \text{and} \quad A_{-1}(\theta) = 0 . \tag{62}$$

With the use of equations 51, 54, 55, 60, 61, and 62, solutions can be found in all energy intervals as follows:

$$K_1(y) = K_o(y) \left[(1 - \alpha^{\frac{1}{1-\alpha}}) - \left(\frac{\alpha^{\frac{1}{1-\alpha}}}{1-\alpha} \ln \alpha y \right) \right] , \tag{63a}$$

and

$$K_2(y) = K_o(y) \left[1-\alpha^{\frac{1}{1-\alpha}} - \theta - \left(\frac{\alpha^{\frac{1}{1-\alpha}}}{1-\alpha} \ln\alpha^2 y \right) \left(1-\alpha^{\frac{1}{1-\alpha}} \right) + \tfrac{1}{2} \left(\frac{\alpha^{\frac{1}{1-\alpha}}}{1-\alpha} \ln\alpha^2 y \right)^2 \right] \tag{63b}$$

For $n \geq 3$, the deviation from asymptotic behavior is small (less than 0.5%), so that no correction from asymptotic behavior is deemed necessary for $n \geq 3$.

From the definitions previously given, it is seen that $K_n(y) = E\,F_n(E)$, where $F_n(E)$ is the collision density in the nth interval. Thus, the correction factor necessary in the appropriate energy interval is given by

$$F_n(E)/F_{as}(E) = C_n(E) \ . \tag{64}$$

From equation 4, it is seen that

$$F_{as}(E) = \text{source strength}/\zeta E \ . \tag{65}$$

Therefore,

$$C_o(E) = \zeta K_o(y) \ , \tag{66a}$$

$$C_1(E) = C_o(E) \left[1 - \alpha^{\frac{1}{1-\alpha}} - \left(\frac{\alpha^{\frac{1}{1-\alpha}}}{1-\alpha} \ln \alpha\, y \right) \right] \ , \tag{66b}$$

$$C_2(E) = C_o(E) \left[1-\alpha^{\frac{1}{1-\alpha}} - \theta - \left(1-\alpha^{\frac{1}{1-\alpha}} \right) \left(\frac{\alpha^{\frac{1}{1-\alpha}}}{1-\alpha} \ln\alpha^2 y \right) + \tfrac{1}{2} \left(\frac{\alpha^{\frac{1}{1-\alpha}}}{1-\alpha} \ln\alpha^2 y \right)^2 \right] \ , \tag{66c}$$

and

$$C_n(E) = 1 \qquad \text{for} \quad n \geq 3. \tag{66d}$$

Equations 40, 41, and 66a-d may be combined to obtain a complete description of the steady-state neutron flux in the model as follows:

$$\phi(x,\ E_o + \Delta E_o/2 \rightarrow E_o - \Delta E_o/2,\ E + \Delta E/2 \rightarrow E - \Delta E/2)$$

= the steady-state neutron flux at the position x in the energy interval $E + \Delta E/2 \rightarrow E - \Delta E/2$ contributed to solely by source

$$\text{neutrons in the energy interval } E_o + \Delta E_o/2 \rightarrow E_o - \Delta E_o/2$$

$$= \frac{\Delta E\, S(E_o + \Delta E_o/2 \rightarrow E - \Delta E_o/2) \exp\left[-x^2/4\tau(E_o,E)\right] C_n(E)}{E\left[\zeta \Sigma_s(E) + \gamma \Sigma_a(E)\right] \sqrt{4\pi\tau(E_o,E)}} , \qquad (67)$$

since

$$\phi(u) = E\, \phi(E) . \qquad (68)$$

In equation 67,

$$S_{norm}(E_o + \Delta E_o/2 \rightarrow E_o - \Delta E_o/2)$$

$$= \int_{E_o - \Delta E_o/2}^{E_o + \Delta E_o/2} 0.76985\, E^{\frac{1}{2}} \exp(-0.775\, E)\, dE , \qquad (69)$$

and

$$\int_0^\infty S(E)\, dE = 1 . \qquad (70)$$

B. Radiation Defect Concentration

A permanent atom (or an interstitial atom) may do one of several things after a short period of time when given energy sufficient for displacement. It may move to an interstitial site (or remain an interstitial in the same or a different site); it may combine with a vacancy; it may move to a boundary or a sink; or it may replace another regular atom (or another interstitial atom).

A vacancy may be annihilated by combination with a moving atom or by

moving to a boundary or a sink.

Interstitials and vacancies may anneal after having come to rest (temporarily) in the lattice. They may do so by recombination or by migration to grain boundaries or to other sinks. This annealing is largely the result of temperature effects present in an irradiated lattice.

The following development will explain the preceding statements in mathematical terms.

The balance equation for interstitial atoms in a lattice may be given by

$$dI/dt = R_{pi} - R_{ai} - R_{ri} , \tag{71}$$

where I is the ratio of interstitial atoms to regular lattice positions, R_{pi} is the fractional production rate for interstitials, R_{ai} is the fractional temperature annealing rate for interstitials, and R_{ri} is the fractional radiation annealing rate for interstitials. The fraction referred to is the ratio of defects to regular lattice positions.

Likewise, the balance equation for vacancies may be given by

$$dV/dt = R_{pv} - R_{av} - R_{rv} , \tag{72}$$

where V is the ratio of vacant lattice positions to regular lattice positions, R_{pv} is the fractional production rate for vacancies, R_{av} is the fractional temperature annealing rate for vacancies, and R_{rv} is the fractional radiation annealing rate for vacancies. The fraction referred to is the ratio of defects to regular lattice positions.

Both R_{pi} and R_{pv} are functions of $\phi(E)$ and of $G(E)$, where $G(E)$ is a cross section for atomic displacement. Therefore, R_{pi} may be given as

$$R_{pi} = P_{iv} P_{is} (1 - I) \int_0^{E_u} \phi(E) G(E) dE, \tag{73}$$

where $(1 - I)$ is the ratio of atoms not displaced to regular lattice positions, P_{iv} is the probability that a moving atom will not combine with an existing vacancy, P_{is} is the probability that a moving atom will not be lost in a sink (other than a vacancy), and the integral term is the fractional rate of production of temporarily displaced atoms.

Likewise, for vacancies, it is found that

$$R_{pv} = P_{vi} P_{vs} (1 - I) \int_0^{E_u} \phi(E) G(E) dE, \tag{74}$$

where P_{vi} is the probability that an existing vacancy will not be filled by a moving atom, and P_{vs} is the probability that an existing vacancy will not be lost in a sink (other than an interstitial).

Equations 73 and 74 give the production rates of interstitials and vacancies and are valid at all times following a displacement.

The quantities R_{ai} and R_{av} apply to those defects which have existed for an appreciable length of time. Each is composed of two terms. One term is governed by the regular temperature annealing which takes place in a lattice. The other term is due to the annealing effect of thermal spikes in the lattice. These terms may be given as

$$R_{ai} = C_1 I^{\gamma_1} \exp(-\epsilon_I/kT) + C_5 I^{\gamma_5} V^{\gamma_7}, \tag{75}$$

where C_1 is a rate constant, γ_1 is an order of reaction, ϵ_I is the interstitial activation energy, k is the Boltzmann constant, T is the absolute temperature, C_5 is a rate constant, γ_5 is an order of reaction, and γ_7 is an order of reaction. The second term is given by

$$R_{av} = C_2 V^{\gamma_2} \exp(-\epsilon_V/kT) + C_6 I^{\gamma_6} V^{\gamma_8} , \tag{76}$$

where the definitions are similar to those in equation 75.

The radiation annealing term for interstitials is given by

$$R_{ri} = (1 - P_{iv} P_{is}) I \int_o^{E_u} \phi(E) G(E) dE . \tag{77}$$

Likewise, the similar term for vacancies is

$$R_{rv} = (1 - P_{iv}) \int_o^{E_l} \phi(E) G(E) dE . \tag{78}$$

Let

$$N(E) = \int_o^{E_u} \phi(E) G(E) dE . \tag{79}$$

When equations 71, 73, 75, 77, and 79 are combined, it is found that

$$dI/dt = (P_{iv} P_{is} - I)N(E) - C_1 I^{\gamma_1} \exp(-\epsilon_I/kT) - C_5 I^{\gamma_5} V^{\gamma_7} . \tag{80}$$

Likewise, for vacancies,

$$dV/dt = (P_{vi} P_{vs} - I P_{vi} P_{vs} + P_{iv} - 1) N(E) - C_2 V^{\gamma_2} \exp(-\epsilon_V/kT) - C_6 I^{\gamma_6} V^{\gamma_8} ; \tag{81}$$

Equations 80 and 81 will be simplified, and individual terms will be more thoroughly investigated before a numerical solution is accomplished.

When considering the terms due to thermal spike annealing, it is known that thermal spikes are of short duration, and each spike includes only a small number of atoms.

According to Seitz and Koehler (75), the temperature of a spherical spike is given by the following relationship:

$$T(r,t') = \frac{Q}{8\pi^{3/2}cd} \frac{1}{(Dt')^{3/2}} \exp(-r^2/4Dt') , \qquad (82)$$

where Q is the energy initially imparted to the spike, c is the specific heat of the material, d is the mass density, D is the heat diffusion coefficient, t' is the time which the spike has been in existence, T is the temperature, and r is the radial distance from the center of the spike.

Equation 82 can be used to obtain a reliable approximation of the situation following a collision where an atom receives energy Q less than the displacement energy, Q_d.

The relationship of interest is the number of atoms in a spike whose temperature exceeds the melting temperature of niobium (as a function of the initial energy received by the spike). To obtain this relationship, equation 82 will be analyzed using the following values for niobium: c is 1.957×10^{12} Mev/gram-$^{\circ}$C, d is 8.4 grams/cm^3, and D is 6.69×10^{-4} cm^2/second. The initial time is taken as 10^{-13} second after the formation of the spike, so that t' in equation 82 becomes

$$t' = t + 10^{-13} . \qquad (82a)$$

This is done so that the temperature does not become infinite at r = 0 and t = 0. Equation 82 thus becomes

$$T(r,t) = \frac{7.897 \times 10^{-17}}{(t + 10^{-13})^{3/2}} \; Q \exp\left(\frac{-374\ r^2}{t + 10^{-13}}\right) \quad , \tag{82b}$$

where Q is to be given in units of ev.

If one differentiates equation 82b with respect to time and keeps in mind that the time can never take on negative values, then it is found that

$$r_T = 1.635 \times 10^{-8} \sqrt{\ln Q} \qquad \text{for } 1.0 \text{ ev} \leq Q \leq 4.5 \text{ ev} \; , \tag{82c}$$

where r_T is the maximum radius of a spherical spike at which the temperature exceeds the melting temperature of niobium (2500°C). Since the atomic density of niobium is 5.45×10^{22} atoms/cm^3, it is readily found that

$$A_m = (\ln Q)^{3/2} \qquad \text{for } 1.0 \text{ ev} \leq Q \leq 4.5 \text{ ev} \; . \tag{82d}$$

A linear approximation is assumed for equation 82d, so that

$$A_m = 0.5255Q - 0.5260 \qquad \text{for } 1.0 \text{ ev} \leq Q \leq 4.5 \text{ ev} \; . \tag{83a}$$

Again, if one differentiates equation 82b with respect to time and only looks at those values of time which are greater than zero, then it is found that

$$r_T = 1.2141 \times 10^{-8} \; Q^{1/3} \qquad \text{for } 4.5 \text{ ev} \leq Q \leq 4, \tag{82e}$$

and

$$A_m = 0.40857 \; Q \qquad \text{for } 4.5 \text{ ev} \leq Q \leq Q_d \; . \tag{83b}$$

It will be assumed that all vacancies anneal by combination with interstitials in that part of a thermal spike whose temperature is greater than the melting temperature of niobium. This assumption is valid since it is assumed that the fraction of interstitials is greater than the fraction of vacancies at all times. Therefore, the annealing terms in each of equations 80 and 81 will be equal, or

$$C_5 I^{\gamma_5} V^{\gamma_7} = C_6 I^{\gamma_6} V^{\gamma_8} . \tag{84}$$

A different expression will now be developed to replace the equal expressions in equation 84.

As neutrons diffuse through the model, some of them will undergo collisions in which they will lose energy less then Q_d. The atoms thus struck, but not displaced, will produce spherical thermal spikes with size dependent upon the energy imparted to the struck atom. Other spherical thermal spikes will be produced by primary, secondary, etc. atoms which strike stationary atoms and give up a part or all of their energy. In a collision with a niobium atom, a neutron can give up energy ranging upwards to 0.0421E, where E is the neutron energy. The fraction of all collisions with neutrons in which the energy transferred is less than Q_d but large enough to produce a spherical spike whose temperature exceeds the melting temperature of niobium is given by

$$F_p = \frac{Q_d - 1.0}{0.0421\ E} \times 10^{-6} . \tag{85}$$

Therefore, the number of collisions producing spherical thermal

spikes of large temperature is given by

$$S_p \, dE = F_p \, \sigma_s(E) \, \phi(E) \, dE \, . \tag{86}$$

The thermal spikes so produced will be called primary spikes because they receive their energy directly from a neutron. Other thermal spikes will be known as secondary spikes because they receive their energy indirectly from neutrons. A secondary spike may be formed when a primary (or secondary, tertiary, etc.) atom strikes a stationary atom and gives it energy insufficient for displacement. A secondary spike may also be produced when a moving atom suddenly comes to rest in the lattice and gives up its kinetic and potential energy.

It will be assumed that there are five times as many secondary spikes produced as there are primary spikes. Therefore, the total number of collisions producing spherical thermal spikes of large temperature is given by

$$S_t \, dE = 1.425(10^{-4})(Q_d - 1.0) \; \sigma_s(E) \, \phi(E) \, dE/E \, . \tag{87}$$

The total number of atoms per unit time contained in spherical spikes whose temperature exceeds the melting temperature of niobium is given by

$$N_s(E) = 1.425(10^{-4})(Q_d - 1.0) \; \bar{A}_m \int_o^{E_u} \sigma_s(E) \, \phi(E) \, dE/E \, , \tag{88a}$$

where $\bar{A}_m$ is the average number of atoms so affected per thermal spike and is given by (from equations 83a-b)

$$\bar{A}_m = \frac{1}{Q_d - 1}\left[\int_{1.0}^{4.5} (0.5255 - 0.526)\, dQ + \int_{4.5}^{Q_d} 0.40857\, Q dQ\right] \quad (89a)$$

$$= 0.204\ (Q_d^{\,2} - 4.503)/(Q_d - 1)\ . \quad (89b)$$

Thus, equation 88a becomes

$$N_s(E) = 2.907(10^{-5})(Q_d^{\,2} - 4.503) \int_o^{E_u} \sigma_s(E)\ \phi(E)\ dE/E\ . \quad (88b)$$

Now, according to preceding statements, the fraction I of the atoms so affected by thermal spikes will be annealed. Therefore, the equal terms in equation 84 can be replaced by $I\ N_s(E)$.

Equations 80 and 81 now become

$$dI/dt = (P_{iv}\ P_{is} - I)N(E) - C_1\ I^{\gamma_1} \exp(-\epsilon_I/kT) - I\ N_s(E) \quad (90)$$

and

$$dV/dt = (P_{vi}\ P_{vs} - IP_{vi}\ P_{vs} + P_{iv} - 1)\ N(E)$$
$$- C_2\ V^{\gamma_2} \exp(-\epsilon_V/kT) - I\ N_s(E)\ . \quad (91)$$

As given previously,

$$N(E) = \int_o^{E_u} \phi(E)\ G(E)\ dE\ , \quad (79)$$

where G(E) is a cross section for atomic displacement. This term will now be examined more closely. Following the argument given by Seitz and Koehler (75),

$$G(E) = \sigma_s(E) \int_{Q_d}^{T_m} g(T'/Q_d)\, dT'/T_m \,, \tag{92}$$

where $\sigma_s(E)$ is the total elastic scattering cross section, T' is the energy of the moving, displaced atom, T_m is the maximum attainable energy of a displaced atom, and $g(T'/Q_d)$ is the number of secondaries produced by a primary with energy T'.

Now $g(T'/Q_d)$ includes the primary atom as well as all those atoms which it displaces. Assuming isotropic atomic collisions, the probability that any atom initially possessing energy T_1' will be found in the energy range T' to $T' + dT'$ after a collision is dT'/T_1'. This is true because the atom may lose any amount of its energy when it collides with a similar atom at rest. Thus, the primary will produce a secondary with energy $T_1' - (T_2' + Q_d)$ if the energy of the first atom is T_2' after the collision. The total number of displaced atoms produced by a given atom of energy $T_1' = x_1\, Q_d$ can be expressed in terms of the number, $g(x_2)$, it will produce after its first collision, and the number, $g(x_1 - x_2 - 1)$, which the secondary atom so produced will itself produce. Here $x_2 = T_2'/Q_d$, where T_2' is the energy of the first atom after its first collision, and $x_1 - x_2 - 1 = s$ is the energy of the first secondary produced. Thus, it is found that

$$g(x_1) = \int_o^{x_1} g(x_2)\, dx_2/x_1 + \int_o^{x_1-1} g(s)ds/x_1 \,. \tag{93}$$

By differentiating equation 93 with respect to x_1, it is found that

$$dg(x_1)/dx_1 = g(x_1 - 1)/x_1 \ . \tag{94}$$

From preceding comments, it is evident that

$$g(x_1) = 1 \qquad \text{for} \quad 0 \leq x_1 \leq 1 \ , \tag{95}$$

since the primary is not able to produce any secondaries if its energy is less than Q_d.

If equation 95 is inserted in the right-hand side of equation 94, it is found that

$$g(x_1) = \ln x_1 + 1 \qquad \text{for} \quad 1 \leq x_1 \leq 2 \ . \tag{96}$$

For $x_1 > 2$, solutions of equation 93 may be obtained by numerical integration, and the solution is found to be nearly linear. The solution is

$$g(x_1) = 0.561 \ (x_1 + 1) \quad \text{for} \quad x_1 > 2 \ . \tag{97}$$

For use in equation 92, $g(x_1)$ will be assumed to have the value given in equation 97 for all values of x_1. This approximation will introduce little error into the solution of equation 92.

Accordingly, equation 92 becomes

$$G(E) = 0.2805 \ \sigma_s(E) \ (2 + T_m/Q_d - 3Q_d/T_m) \ , \tag{98}$$

and equation 79 becomes

$$N(E) = 0.2805 \int_o^{E_u} (2 + T_m/Q_d - 3Q_d/T_m) \ \sigma_s(E) \ \phi(E) \ dE \ . \tag{99}$$

By inserting equations 88b and 99 into equations 90 and 91, it is found that

$$dI/dt = 0.2805(P_{iv}\,P_{is} - I)\int_o^{E_u}(2+T_m/Q_d-3Q_d/T_m)\,\sigma_s(E)\,\phi(E)\,dE$$

$$- 2.907(10^{-5})\,I\,(Q_d^{\,2} - 4.503)\int_o^{E_u}\sigma_s(E)\,\phi(E)\,dE/E$$

$$- C_1\,I^{\gamma_1}\exp(-\epsilon_I/kT)\,, \qquad (100)$$

and

$$dV/dt =$$

$$0.2805\,(P_{vi}P_{vs}-IP_{vi}P_{vs}+P_{iv}-1)\int_o^{E_u}(2+T_m/Q_d-3Q_d/T_m)\sigma_s(E)\phi(E)dE$$

$$-2.907(10^{-5})\,I\,(Q_d^{\,2}-4.503)\int_o^{E_u}\sigma_s(E)\,\phi(E)\,dE/E$$

$$-C_2\,V^{\gamma_2}\exp(-\epsilon_V/kT)\,. \qquad (101)$$

VI. SOLUTION OF EQUATIONS

Solutions for equations 100 and 101 will now be developed where the flux is described by equations 40, 66a-d, 67, and 69. As a first step in the solution, values must be determined for some of the terms in the equations. The terms α, ζ, γ, and θ are constants for any given material. These values for niobium are all functions only of atomic weight and are

$$\alpha = 0.95786 \ , \tag{102a}$$

$$\zeta = 0.021373, \tag{102b}$$

$$\gamma = 0.014301, \tag{102c}$$

and

$$\theta = 0.36787 \ . \tag{102d}$$

If the above values are inserted in equations 51 and 66a-c, it is found that

$$C_o(E) = (E_o/E)^{22.730} \left[0.50719\right] \ , \tag{103a}$$

$$C_1(E) = (E_o/E)^{22.730} \left[0.32461-4.3328 \left\{\ln(.95786E_o/E)\right\}\right] \ , \tag{103b}$$

and

$$C_2(E) = (E_o/E)^{22.730} \left[0.13803-2.7730 \left\{\ln(.91750\ E_o/E)\right\} + 18.507\ (\ln .91750\ E_o/E)^2\right] \ . \tag{103c}$$

With the proper values inserted, equation 67 becomes

$$\phi(x,\ E_o + \Delta E_o/2 \rightarrow E_o - \Delta E_o/2,\ E + \Delta E/2 \rightarrow E - \Delta E/2)$$

$$= \frac{0.76985\ \Delta E\ C_n(E) \left[\int_{E_o-\Delta E_o/2}^{E_o+\Delta E_o/2} E^{\frac{1}{2}}\exp(-0.775E)dE\right] \exp\left[-x^2/4\tau(E_o,E)\right]}{E\left[.021373\ \Sigma_s(E) + .014301\ \Sigma_a(E)\right]\sqrt{4\pi\tau(E_o,E)}}\ , \quad (104)$$

where

$$\tau(E_o,E) = \int_E^{E_o} \frac{D(E)}{\left[.021373\ \Sigma_s(E) + .014301\ \Sigma_a(E)\right]} \cdot \frac{dE}{E}\ . \quad (105)$$

The diffusion coefficient is given by

$$D(E) = \frac{1}{3\left[\Sigma_s(E) + \Sigma_a(E)\right]\left[1 - \bar{\mu}_o\right]\left[1 + \frac{\Sigma_a(E)}{\Sigma_s(E)+\Sigma_a(E)}\left(\frac{\bar{\mu}_o}{1-\bar{\mu}_o} - \frac{4}{5}\right)\right]}\ , \quad (106)$$

where

$$\bar{\mu}_o = 2/3A = 0.0071754\ . \quad (107)$$

Hughes and Schwartz (42) give graphical representations of $\sigma_s(E)$ and $\sigma_a(E)$. The graphical values for niobium may be approximated by mathematical expressions. These are found to be

$$\sigma_s(E) = 5.2 \text{ barns} \qquad \text{for all } E, \quad (108)$$

and

$$\sigma_a(E) = 1.2 \text{ barns} \qquad \text{for } 0 < E \leq .0032378 \text{ Mev} \quad (109a)$$

$$= 0.0369335E^{-0.60719} \qquad \text{for } E > .0032378 \text{ Mev}\ . \quad (109b)$$

For niobium it is found that $\Sigma = N\sigma = 0.05447\sigma$, where σ is expressed in barns.

Values are found for $\phi(x,E_o,E)$ using a numerical solution. This is done by dividing the energy spectrum from 0 to 10 Mev into eleven energy groups as shown in Table 1. There will be source neutrons in the first ten energy groups, and flux will be present in groups two through eleven, since source neutrons produced in a certain group contribute only to the flux in groups of lower energy.

Table 1. Energies and sources for numerical solution

Energy group	E_{upper} Mev	E_{lower} Mev	E_{avg} Mev	Normalized source
1	10	9	9.5	0.00155
2	9	8	8.5	0.00317
3	8	7	7.5	0.00647
4	7	6	6.5	0.01306
5	6	5	5.5	0.02604
6	5	4	4.5	0.05107
7	4	3	3.5	0.09749
8	3	2	2.5	0.17804
9	2	1	1.5	0.29569
10	1	0.0032378	0.5016189	0.32742
11	0.0032378	thermal	0.0016189	-------

An approximate correction for the non-asymptotic case near source energies can be made by using the average values of the $C_n(E)$'s in their appropriate ranges. These are found to be

$$\bar{C}_o(E) = 0.85575 \quad \text{for} \quad 0.95786E_o < E < E_o \,, \tag{111a}$$

$$\bar{C}_1(E) = 0.97652 \quad \text{for} \quad 0.91750E_o \leq E \leq 0.95786E_o \,, \tag{111b}$$

and

$$\bar{C}_2(E) = 0.99670 \quad \text{for} \quad 0.87884E_o \leq E \leq 0.91750E_o \,. \tag{111c}$$

In Table 2 are found the macroscopic cross sections for each energy group.

Table 2. Macroscopic cross sections

Energy group	Σ_a cm^{-1}	Σ_s cm^{-1}
1	0.000513	0.2832
2	0.000549	0.2832
3	0.000592	0.2832
4	0.000645	0.2832
5	0.000714	0.2832
6	0.000808	0.2832
7	0.000940	0.2832
8	0.001153	0.2832
9	0.001573	0.2832
10	0.003058	0.2832
11	0.065364	0.2832

In Appendix A will be found tabulated values for $\tau(E_o,E)$, $\sqrt{\tau(E_o,E)}$, and $\phi(x,E_o,E)$, all for a unit total source.

Equations 100 and 101 will now be examined. As given previously, Q_d is the displacement energy for a niobium atom in a lattice position. It is evident that this quantity varies according to several factors. Experimental methods have been used to determine average values for Q_d in various metals. A value for niobium is determined from the literature (73) to be

$$Q_d = 25 \text{ ev} . \tag{112}$$

As previously given, T_m is the maximum attainable energy of a primary displaced atom. This is dependent upon the neutron energy in the following manner:

$$\begin{aligned} T_m &= (1 - \alpha)E - Q_d \\ &= (0.04214E - 25 \times 10^{-6}) \text{ Mev} . \end{aligned} \tag{113}$$

The interstitial and vacancy activation energies of self-diffusion, ϵ_I and ϵ_V, are given in the literature (3, 11, 52, and 54) (for $0^\circ C$ temperature) as

$$\epsilon_I = 0.7 \text{ ev} , \tag{114a}$$

and

$$\epsilon_V = 1.3 \text{ ev} . \tag{114b}$$

With the proper values inserted for the Boltzmann constant and with $T = 273.2^\circ K$, it is found that

$$\exp(-\epsilon_I/kT) = 1.2136 \times 10^{-13} , \tag{115a}$$

and

$$\exp(-\epsilon_V/kT) = 9.9108 \times 10^{-25} . \tag{115b}$$

A typical order of reaction for vacancies is given in the literature (11 and 75) as

$$\gamma_2 = 2.5 . \tag{116a}$$

Since there are assumed to be more interstitials present than vacancies, the order of reaction for interstitials may be somewhat less than that for vacancies. Therefore, it will be assumed that

$$\gamma_1 = 2.0 . \tag{116b}$$

In looking at the four probabilities in equations 100 and 101, it is evident from the definitions given that P_{iv} is equal to P_{vi}. P_{iv} must have a value between zero and unity. It is unlikely that it would be zero because some of the moving atoms will remain as interstitials and

others will be lost to sinks. This probability will not equal unity because there is always chance for combination between a moving atom and a vacancy if there are any vacancies present. P_{iv} is dependent upon V, I, and upon the concentration of sinks present. However, it is probably more dependent upon V than upon the other two. P_{iv} equals one only when V equals zero (at the beginning of an irradiation), and it decreases with increasing V. It is evident that P_{iv} can never be zero, and its value is no doubt asymptotic to some value between zero and unity for long exposure times. Therefore, for purposes of illustration in an example, the following value will be assigned to P_{iv}. It is considered to be reasonable for long exposure times:

$$P_{iv} = P_{vi} = 0.7 \ . \tag{117}$$

Now P_{is}, the probability that a moving atom will not be lost in a sink (including a crystal boundary), will also lie between zero and unity. However, it can never equal unity because there will always be crystal boundaries present, even at the start of irradiation. The concentration of sinks will probably be less than the concentration of vacancies, so that P_{is} will be larger than P_{iv}. Thus, the following value will be assigned to P_{is} for purposes of illustration:

$$P_{is} = 0.9 \ . \tag{118}$$

The probability that a moving atom will (temporarily) become an interstitial is 0.6 (from equations 117 and 118).

The probability that an existing vacancy will not be lost in a sink

(including a crystal boundary), P_{vs}, also has a value which lies between zero and unity. With the use of reasoning similar to the preceding, it is assumed that

$$P_{vs} = 0.8 \ . \tag{119}$$

This value for P_{vs} is taken to be somewhat smaller than the value for P_{is}, since there are assumed to be fewer vacancies present than interstitials, which would tend to indicate that more of them are lost than is the case for interstitials. The probability that an existing (temporary) vacancy will not be immediately lost is found to be 0.5 (from equations 117 and 119).

With the preceding values inserted into equations 100 and 101, it is found that

$$dI/dt = 0.2805(0.63-I)\int_o^{E_u}\left[1+1.6856\times10^3E-\frac{3}{1.6856\times10^3E-1}\right]\sigma_s(E)\phi(E)dE$$

$$- 1.2136\times10^{-13}C_1I^2-0.0180377\ I\int_o^{E_u}\sigma_s(E)\phi(E)dE/E \ , \tag{120}$$

and

$$dV/dt = 0.1571(0.4643-I)\int_o^{E_u}\left[1+1.6856\times10^3E-\frac{3}{1.6856\times10^3E-1}\right]\sigma_s(E)\phi(E)dE$$

$$- 9.9108\times10^{-25}C_2V^{2.5}-0.0180377\ I\int_o^{E_u}\sigma_s(E)\phi(E)dE/E \ . \tag{121}$$

Equations 120 and 121 are solved for various neutron-source strengths. Four initial and boundedness conditions are used, being

1) $I = 0 , t = 0 ,$ (122a)

2) $V = 0 , t = 0 ,$ (122b)

3) $dI/dt = 0 , I = .02 ,$ (122c)

and

4) $dV/dt = 0 , V = .01 .$ (122d)

The values for I and V in 122c-d are reasonable values (assumed) which may exist at an infinite irradiation time. By fixing these asymptotic values, the shapes of the curves of radiation defect concentrations versus time are obtained.

Tabulated values for

$$F_1(x,E) = \int_o^{E_u} \left[1+1.6856\times10^3 E - \frac{3}{1.6856\times10^3 E-1}\right]\sigma_s(E)\phi(x,E)dE \quad (123a)$$

and

$$F_2(x,E) = \int_o^{E_u} \sigma_s(E)\phi(x,E)dE/E \quad (123b)$$

for a source strength of unity are presented in Appendix B.

In Table 3 are presented the constants for the equations of I as a function of time as given by the following relationship:

$$I = \frac{e^{a't} - 1}{50\, e^{a't} + b} . \quad (124)$$

The constants are given for various source strengths and distances from the source.

In Table 4 are presented the constants for the equations of dV/dt as a function of time as given by the following relationship:

$$dV/dt = m - n' I(t) - p' V^{2.5} . \quad (125)$$

The constants given are for the same source strengths and distances as in Table 3.

Table 3. Constants for equation 124

Source n/cm^2-sec	Distance x cm	a'	b
10^{12}	0	1.14223×10^{-6}	48.36426
10^{12}	1	1.09557×10^{-6}	48.36221
10^{12}	2	9.88282×10^{-7}	48.35676
10^{12}	3	8.70274×10^{-7}	48.34924
10^{12}	4	7.62996×10^{-7}	48.34042
10^{12}	5	6.71403×10^{-7}	48.33071
10^{12}	10	3.85664×10^{-7}	48.27200
10^{12}	15	2.52183×10^{-7}	48.20256
10^{11}	20	1.80460×10^{-8}	48.12850
3×10^{11}	20	5.41380×10^{-8}	48.12850
10^{12}	20	1.80460×10^{-7}	48.12850
3×10^{12}	20	5.41380×10^{-7}	48.12850
10^{13}	20	1.80460×10^{-6}	48.12850
10^{12}	30	1.13078×10^{-7}	47.99928
10^{12}	40	8.28174×10^{-8}	47.91585
10^{12}	50	6.02690×10^{-8}	47.83202
10^{12}	75	2.06076×10^{-8}	47.43084
10^{12}	100	4.59661×10^{-9}	46.31002

Equation 124 expresses I as a function of time without approximation.

Equation 125 may be solved approximately to obtain values of V as a function of time. This solution may be accomplished by rearranging equation 125 as

$$\int_{V_i}^{V_{i+1}} dV = m \int_{t_i}^{t_{i+1}} dt - n' \int_{t_i}^{t_{i+1}} \left(\frac{e^{a't}-1}{50e^{a't}+b} \right) dt - p' \int_{t_i}^{t_{i+1}} V^{2.5} dt \quad (126a)$$

Equation 126a in expanded form becomes

$$V_{i+1} = V_i + (m+n'/b)(t_{i+1}-t_i)$$

$$+(n'/a')(.02+1/b)\ln\left|(e^{a't_i}+0.02b)/(e^{a't_{i+1}}+0.02b)\right|-p'\int_{t_i}^{t_{i+1}} V^{2.5}dt. \qquad (126b)$$

Table 4. Constants for equation 125

Source n/cm^2-sec	Dis. x cm	m	n'	p'
10^{12}	0	4.79313×10^{-9}	1.08858×10^{-8}	4.57542×10^{-4}
10^{12}	1	4.59740×10^{-9}	1.04641×10^{-8}	4.38812×10^{-4}
10^{12}	2	4.14742×10^{-9}	9.49465×10^{-9}	3.95753×10^{-4}
10^{12}	3	3.65247×10^{-9}	8.42810×10^{-9}	3.48390×10^{-4}
10^{12}	4	3.20252×10^{-9}	7.45829×10^{-9}	3.05335×10^{-4}
10^{12}	5	2.81835×10^{-9}	6.62994×10^{-9}	2.68576×10^{-4}
10^{12}	10	1.61987×10^{-9}	4.04100×10^{-9}	1.53905×10^{-4}
10^{12}	15	1.05997×10^{-9}	2.82258×10^{-9}	1.00352×10^{-4}
10^{11}	20	7.59080×10^{-11}	2.15754×10^{-10}	7.15929×10^{-6}
3×10^{11}	20	2.27724×10^{-10}	6.47262×10^{-10}	2.14779×10^{-5}
10^{12}	20	7.59080×10^{-10}	2.15754×10^{-9}	7.15929×10^{-5}
3×10^{12}	20	2.27724×10^{-9}	6.47262×10^{-9}	2.14779×10^{-4}
10^{13}	20	7.59080×10^{-9}	2.15754×10^{-8}	7.15929×10^{-4}
10^{12}	30	4.76275×10^{-10}	1.50282×10^{-9}	4.46218×10^{-5}
10^{12}	40	3.49116×10^{-10}	1.17216×10^{-9}	3.25673×10^{-5}
10^{12}	50	2.54281×10^{-10}	9.05388×10^{-10}	2.36174×10^{-5}
10^{12}	75	8.73037×10^{-11}	3.95707×10^{-10}	7.93896×10^{-6}
10^{12}	100	1.97000×10^{-11}	1.42778×10^{-10}	1.68444×10^{-7}

To evaluate the integral term in equation 126b, a linear relationship between V and t in the interval t_i to t_{i+1} is assumed, or

$$V = V_i + (V_{i+1} - V_i)(t - t_i)/(t_{i+1} - t_i) . \qquad (127)$$

When equation 127 is inserted into the integral term of equation 126b and the integration is carried out, it is found that

$$p' \int_{t_i}^{t_{i+1}} v^{2.5} dt = (2p/7)(t_{i+1}-t_i)(V_{i+1}^{7/2} - V_i^{7/2})/(V_{i+1} - V_i) \quad . \quad (128)$$

Equation 126b is then solved by an iterative process where

$$(V_{i+1})_1 = V_i + (m' + n'/b)\ (t_{i+1} - t_i)$$

$$+ (n'/a')\ (0.02 + 1/b)\ \ln\ (e^{a't_i} + 0.02)/(e^{a't_{i+1}} + 0.02b), \quad (126c)$$

and

$$(V_{i+1})_{j+1} = (V_{i+1})_1 - (2p'/7)\ (t_{i+1} - t_i)\ \left[(V_{i+1})_j^{7/2} - V_i^{7/2}\right]$$

$$/\left[(V_{i+1})_j - V_i\right] \quad . \quad (126d)$$

The iteration in equation 126d is continued until

$$\left|(V_{i+1})_{j+1} - (V_{i+1})_j\right| < \delta' \quad . \quad (126e)$$

A FORTRAN program for the solution of equations 124 and 125 is seen in Appendix C. On following pages appear graphical representations of IBM-704 solutions for these equations.

VII. RESULTS

The results of this study are summarized in equations 100, 101, and 122a-d (seen on previous pages). These equations give the interstitial and vacancy fractions as functions of time in a niobium lattice in which there exists a steady-state neutron flux. The equations are solved in the preceding section using representative values (assumed where necessary). The solutions are depicted graphically in Figures 1-4 on the following pages.

Figure 1. Interstitial fraction, I, versus time at various distances from a plane source with a strength of 10^{12} neutrons per cm^2 per second

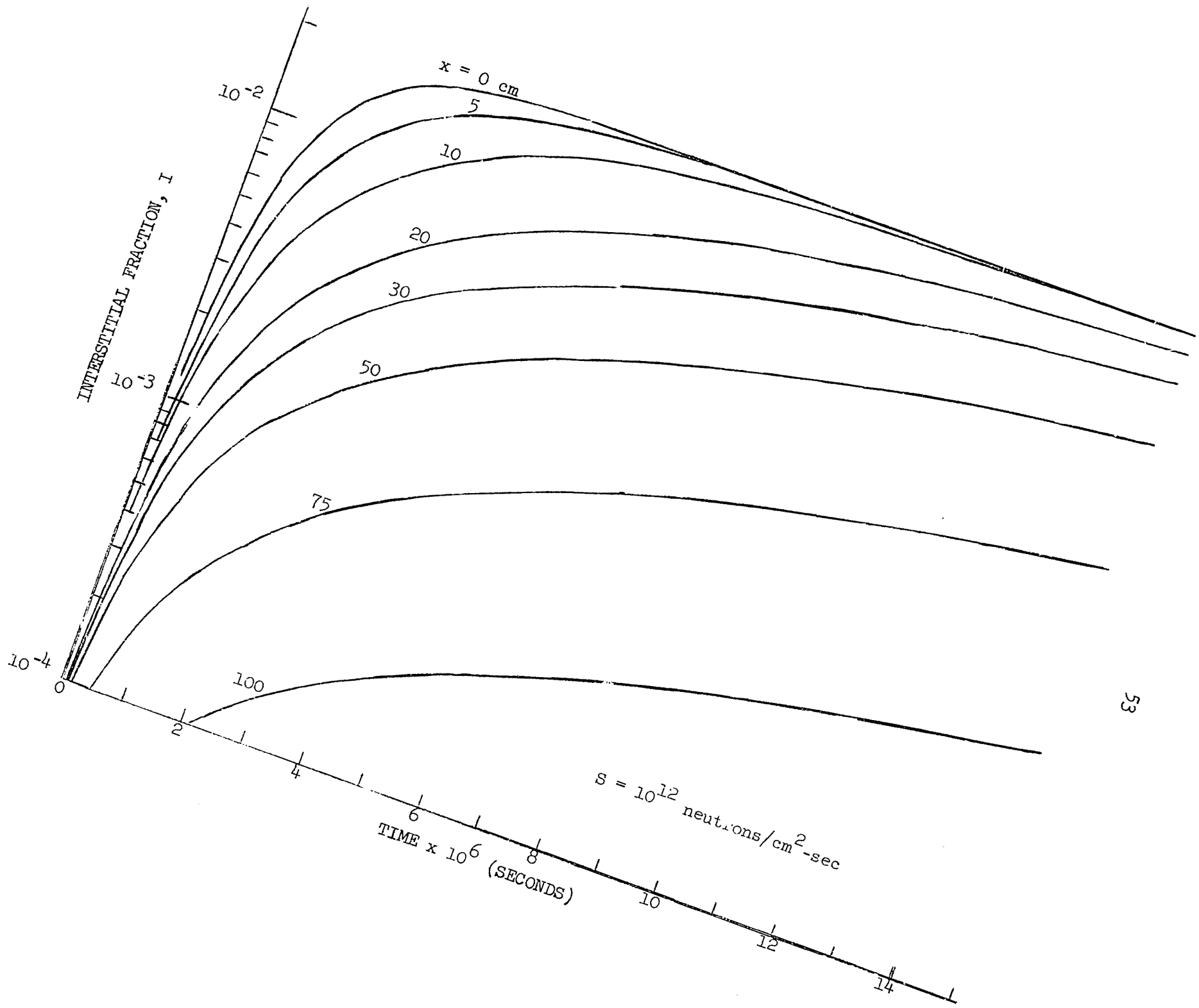

INTERSTITIAL FRACTION, I
1
10^{-2}
10^{-3}
10^{-4}
0
2
4
6
8
10
12
14
TIME x 10^6 (SECONDS)
x = 0 cm
5
10
20
30
50
75
100
S = 10^{12} neutrons/cm^2-sec

Figure 2. Vacancy fraction, V, versus time at various distances from a plane source with a strength of 10^{12} neutrons per cm^2 per second

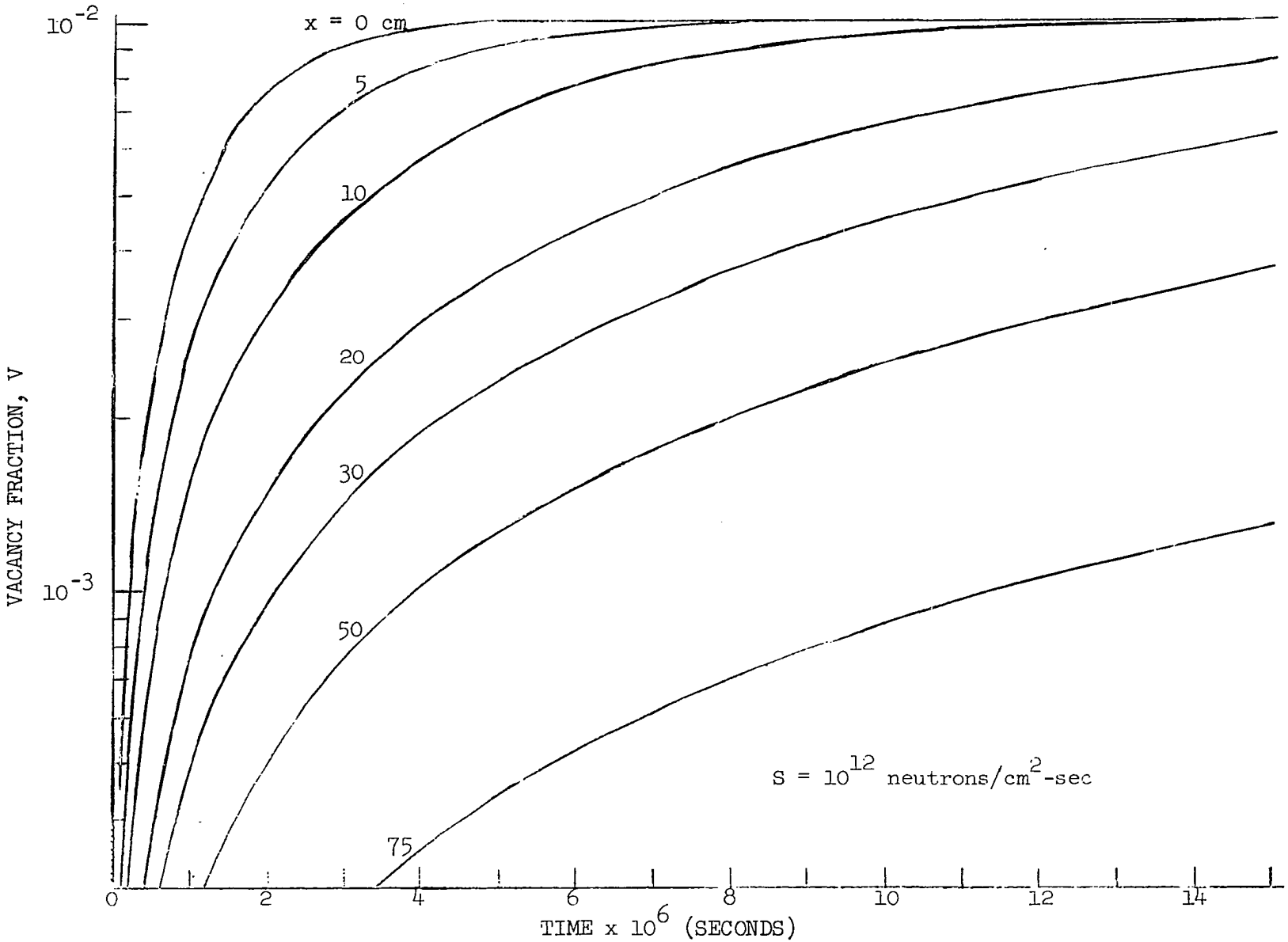

VACANCY FRACTION, V
10^{-2}
10^{-3}
x = 0 cm
5
10
20
30
50
75
S = 10^{12} neutrons/cm^2-sec
0
2
4
6
8
10
12
14
TIME x 10^6 (SECONDS)

Figure 3. Interstitial fraction, I, versus time at a distance of twenty centimeters from plane sources of various strengths

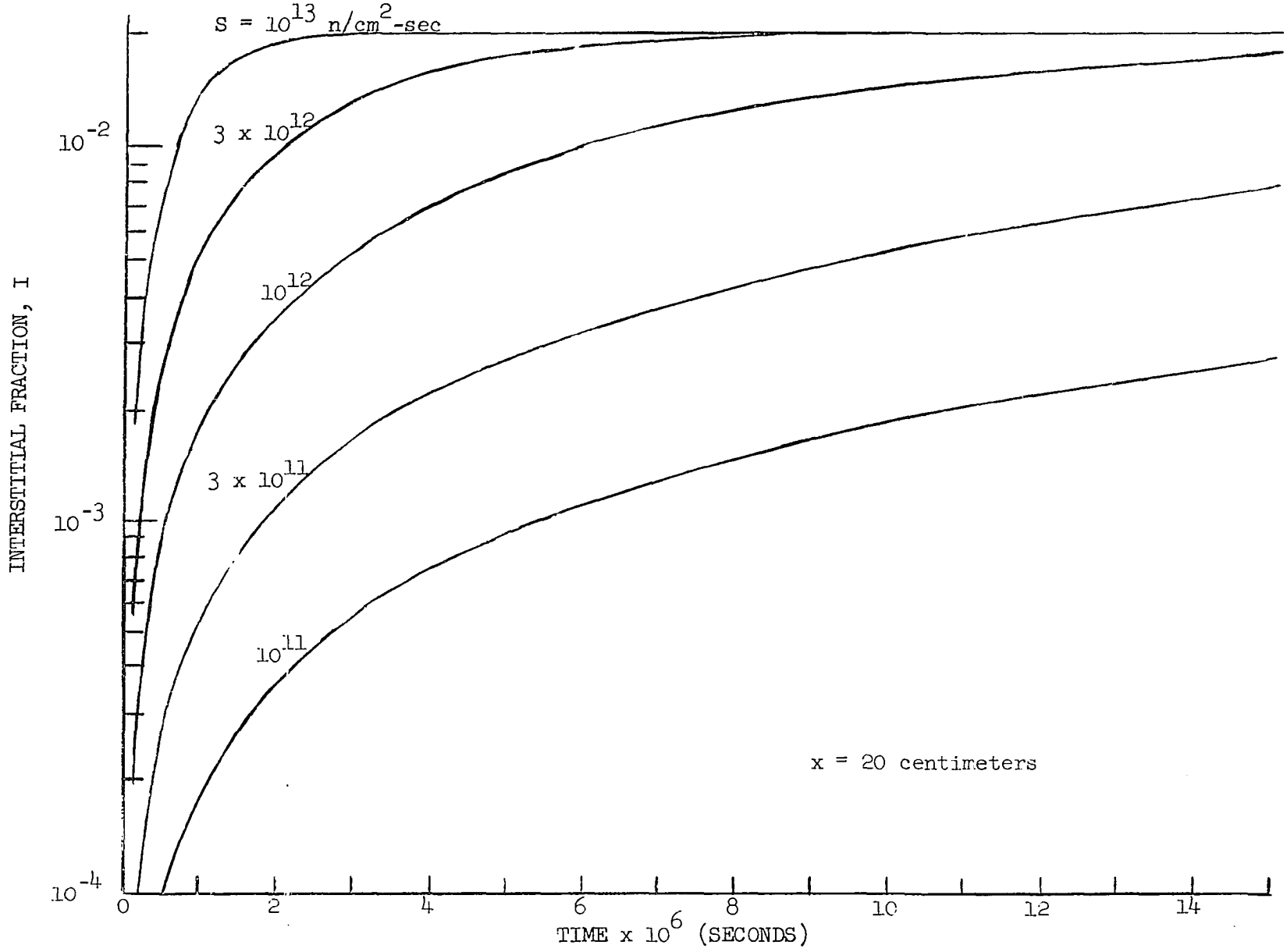
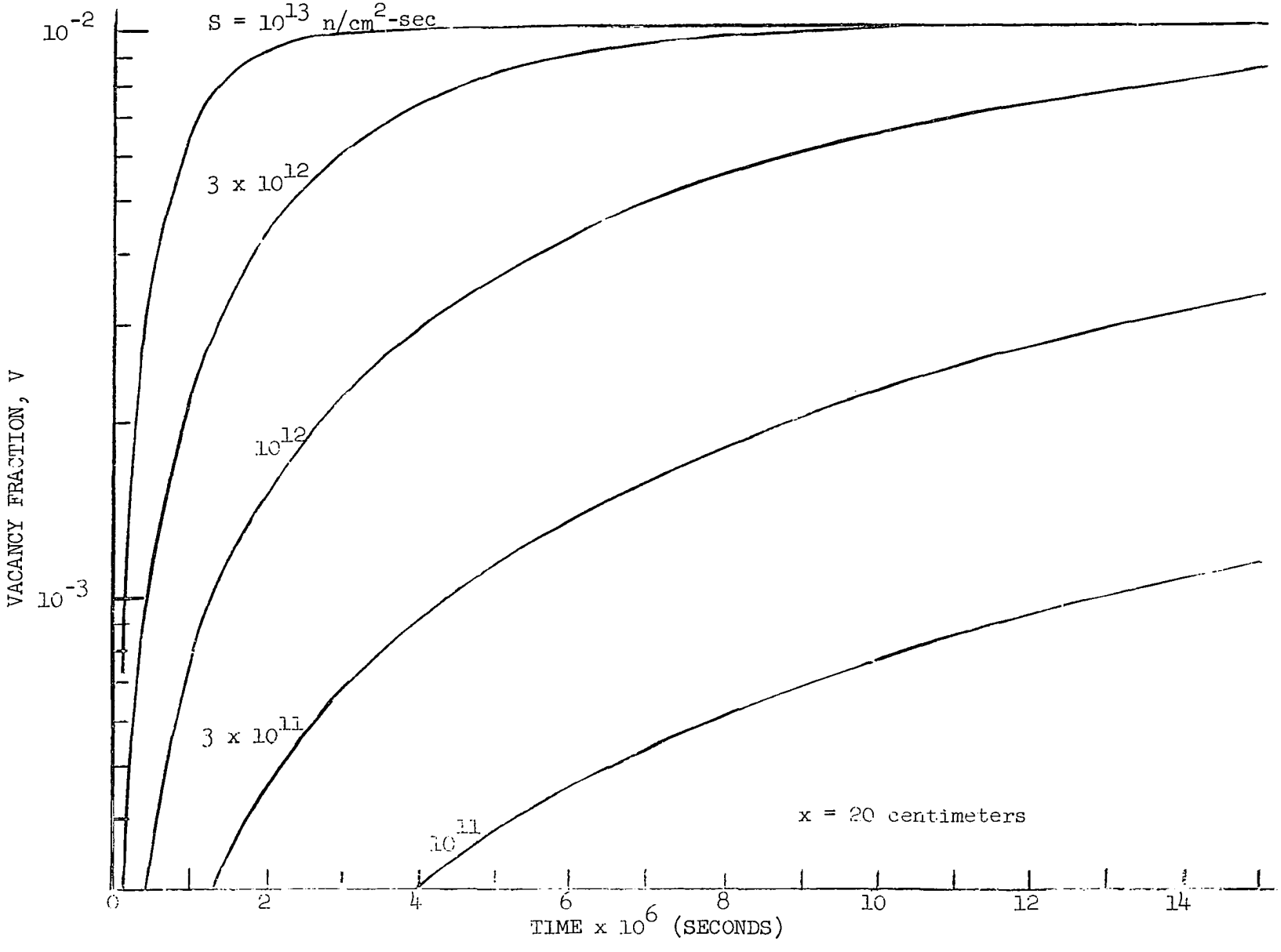

S = 10^13 n/cm^2-sec
3 x 10^12
10^12
3 x 10^11
10^11
x = 20 centimeters
INTERSTITIAL FRACTION, I
10^-2
10^-3
10^-4
0
2
4
6
8
10
12
14
TIME x 10^6 (SECONDS)

Figure 4. Vacancy fraction, V, versus time at a distance of twenty centimeters from plane sources of various strengths


10^{-2}
10^{-3}
VACANCY FRACTION, V
S = 10^{13} n/cm^2-sec
3 x 10^{12}
10^{12}
3 x 10^{11}
10^{11}
x = 20 centimeters
0
2
4
6
8
10
12
14
TIME x 10^6 (SECONDS)

VIII. SUMMARY

The accumulation of neutron-induced radiation defects in niobium metal (in this case interstitial atoms and vacant lattice sites) can be described in the following manner. The rate of accumulation is equal to the rate of production minus the recovery rate. The rate of production is dependent upon the flux (energy dependent), the defect concentration, neutron parameters, and metal parameters. The recovery rate is composed of two terms--temperature annealing and radiation-induced annealing. Temperature annealing is dependent upon the temperature, type of defect, defect concentration, and metal parameters. Radiation-induced annealing is dependent upon the flux (energy dependent), the defect concentration, neutron parameters, and metal parameters.

For a given neutron flux, the fractional concentration of defects produced is dependent to a large extent on the energy of the neutrons. This dependence has been included in the development of the equations.

Fractional defect concentrations (as defined in this dissertation) saturate at some level. The equations and definitions describing the fractional concentrations of defects support this conclusion as does the literature (3).

IX. RECOMMENDATIONS FOR FURTHER STUDY

It would be advisable to develop an extensive computer code which could determine the effects on defect concentrations caused by varying a considerable number of parameters. Single values were assumed for some of the parameters in this study.

It would also be of interest to determine accurate values for some of the assumed parameters used in the study, either through extensive analytical work or by experimental means.

A similar study could be done using fission fragments instead of neutrons as the bombarding particles.

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XII. APPENDIX A: VALUES OF NEUTRON AGE AND FLUX PER UNIT ENERGY (FROM EQUATIONS 104 AND 105)

Table 5. Values of neutron age in niobium (square root in parenthesis)

E_o, Mev →	9.5	8.5	7.5	6.5	5.5
E, Mev					
8.5	0.5933 (0.7703)				
7.5	1.3642 (1.1680)	0.7709 (0.8780)			
6.5	2.5176 (1.5867)	1.9243 (1.3872)	1.1534 (1.0740)		
5.5	4.3560 (2.0871)	3.7627 (1.9398)	2.9919 (1.7297)	1.8384 (1.3559)	
4.5	7.5525 (2.7482)	6.9592 (2.6380)	6.1883 (2.4876)	5.0349 (2.2439)	3.1965 (1.7879)
3.5	13.8671 (3.7239)	13.2738 (3.6433)	12.5030 (3.5360)	11.3495 (3.3689)	9.5111 (3.0840)
2.5	29.2117 (5.4048)	28.6184 (5.3496)	27.8475 (5.2771)	26.6941 (5.1666)	24.8557 (4.9855)
1.5	84.9068 (9.2145)	84.3135 (9.1822)	83.5426 (9.1402)	82.3892 (9.0768)	80.5507 (8.9750)
0.5016189	776.0479 (27.8576)	775.4546 (27.8470)	774.6837 (27.8331)	773.5303 (27.8124)	771.6918 (27.7793)
0.0016189	1789.3737 (42.3010)	1788.7804 (42.2940)	1788.0095 (42.2849)	1786.8561 (42.2712)	1785.0176 (42.2495)

E_o, Mev →	4.5	3.5	2.5	1.5	0.5016189
E, Mev					
3.5	6.3146 (2.5129)				
2.5	21.6592 (4.6539)	15.3446 (3.9172)			
1.5	77.3543 (8.7951)	71.0396 (8.4285)	55.6951 (7.4629)		
0.5016189	768.4954 (27.7217)	762.1807 (27.6076)	746.8362 (27.3283)	691.1411 (26.2896)	
0.0016189	1781.8212 (42.2116)	1775.5065 (42.1368)	1760.1620 (41.9543)	1704.4669 (41.2852)	1013.3258 (31.8328)

Table 6. Flux per unit energy in niobium for a unit plane source

x, cm →	0	1	2	3	4	5	10
E, Mev							
8.5	0.0079	0.0052	0.0015	0.0002	0.0000	0.0000	0.0000
7.5	0.0251	0.0188	0.0082	0.0022	0.0004	0.0001	0.0000
6.5	0.0514	0.0430	0.0255	0.0112	0.0039	0.0012	0.0000
5.5	0.1013	0.0907	0.0654	0.0387	0.0194	0.0086	0.0000
4.5	0.1939	0.1820	0.1505	0.1104	0.0725	0.0432	0.0012
3.5	0.3605	0.3489	0.3165	0.2694	0.2156	0.1627	0.0192
2.5	0.6468	0.6380	0.6124	0.5723	0.5201	0.4612	0.1721
1.5	1.1062	1.1019	1.0890	1.0680	1.0392	1.0032	0.7489
0.5016189	1.8700	1.8692	1.8674	1.8642	1.8597	1.8539	1.8069
0.0016189	505.7254	505.6326	505.3541	504.8898	504.2399	503.4043	496.5454
x, cm →	15	20	30	40	50	75	100
E, Mev							
8.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.5	0.0009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2.5	0.0370	0.0052	0.0000	0.0000	0.0000	0.0000	0.0000
1.5	0.4620	0.2376	0.0375	0.0032	0.0002	0.0000	0.0000
0.5016189	1.7314	1.6297	1.3721	1.0781	0.7914	0.2712	0.0608
0.0016189	485.3170	470.0833	429.1135	378.0948	321.9095	186.9742	90.3864

XIII. APPENDIX B: VALUES OF $F_1(x,E)$ AND $F_2(x,E)$ (FROM EQUATIONS 123a-b)[2]

Table 7. Values of 10^{20} $F_1(x,E)$ for a unit plane source

x, cm →	0	1	2	3	4	5	10
E, Mev							
8.5	0.0590	0.0387	0.0109	0.0013	0.0001	0.0000	0.0000
7.5	0.1650	0.1238	0.0537	0.0147	0.0029	0.0005	0.0000
6.5	0.2928	0.2449	0.1451	0.0638	0.0222	0.0066	0.0000
5.5	0.4885	0.4374	0.3154	0.1866	0.0934	0.0416	0.0002
4.5	0.7650	0.7178	0.5937	0.4354	0.2859	0.1703	0.0047
3.5	1.1061	1.0707	0.9712	0.8267	0.6614	0.4993	0.0590
2.5	1.4176	1.3984	1.3424	1.2545	1.1399	1.0108	0.3773
1.5	1.4550	1.4493	1.4324	1.4047	1.3669	1.3195	0.9850
0.5016189	0.8205	0.8202	0.8194	0.8179	0.8160	0.8134	0.7928
0.0016189	0.0019	0.0019	0.0018	0.0018	0.0018	0.0018	0.0018
x, cm →	15	20	30	40	50	75	100
E, Mev							
8.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
7.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4.5	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3.5	0.0029	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
2.5	0.0812	0.0113	0.0001	0.0000	0.0000	0.0000	0.0000
1.5	0.6077	0.3125	0.0493	0.0042	0.0002	0.0000	0.0000
0.5016189	0.7597	0.7151	0.6020	0.4730	0.3472	0.1190	0.0267
0.0016189	0.0018	0.0017	0.0016	0.0014	0.0012	0.0007	0.0003

Table 8. Values of 10^{24} $F_2(x,E)$ for a unit plane source

x, cm →	0	1	2	3	4	5	10
E, Mev							
8.5	0.005	0.003	0.001	0.000	0.000	0.000	0.000
7.5	0.017	0.013	0.006	0.002	0.000	0.000	0.000
6.5	0.041	0.034	0.020	0.009	0.003	0.001	0.000
5.5	0.096	0.086	0.062	0.037	0.018	0.008	0.000
4.5	0.225	0.211	0.175	0.128	0.084	0.050	0.001
3.5	0.539	0.522	0.473	0.403	0.322	0.243	0.029
2.5	1.364	1.345	1.291	1.207	1.097	0.972	0.363
1.5	3.987	3.972	3.925	3.849	3.746	3.616	2.699
0.5016189	55.746	55.724	55.669	55.573	55.439	55.267	53.864
0.0016189	31119.182	31113.469	31096.329	31067.763	31027.770	30976.351	30554.301
x, cm →	15	20	30	40	50	75	100
E, Mev							
8.5	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7.5	0.000	0.000	0.000	0.000	0.000	0.000	0.000
6.5	0.000	0.000	0.000	0.000	0.000	0.000	0.000
5.5	0.000	0.000	0.000	0.000	0.000	0.000	0.000
4.5	0.000	0.000	0.000	0.000	0.000	0.000	0.000
3.5	0.001	0.000	0.000	0.000	0.000	0.000	0.000
2.5	0.078	0.011	0.000	0.000	0.000	0.000	0.000
1.5	1.665	0.856	0.135	0.012	0.001	0.000	0.000
0.5016189	51.615	48.583	40.905	32.139	23.591	8.085	1.812
0.0016189	29863.374	28925.988	26404.964	23265.592	19808.298	11505.221	5561.815

XIV. APPENDIX C: IBM-704 FORTRAN PROGRAM

Table 9. Parameters for IBM-704 program

Symbol	Description	Type
INPUT		
N	Problem number	Integer
IMAX	Total number of points for which output values are computed	Integer
D	Convergence criterion from equation 126e	Floating point
DT	Time increment, $t_{i+1} - t_i$	Floating point
E	$m + n'/b$ from equation 126c	Floating point
F	a' from equation 126c	Floating point
G	$(n'/a')\ (0.02 + 1/b)$ from equation 126c	Floating point
P	0.02b from equation 126c	Floating point
Q	$2p'/7$ from equation 126d	Floating point
OUTPUT		
T	Time	Floating point
Z	Interstitial fraction	Floating point
V	Vacancy fraction	Floating point

Table 10. IBM-704 program: Solutions to Kristianson Nonlinear Equation

STATEMENT NUMBER	FORTRAN STATEMENT
1	DIMENSIØN T(10000),V(10000),Z(10000)
5	FØRMAT(6E12.6/E12.6)
10	FØRMAT(I2,I4)
15	READ INPUT TAPE 7,10,N,IMAX
20	WRITE ØUTPUT TAPE 6,25
25	FØRMAT(44H1SØLUTIØNS TØ KRISTIANSØN NØNLINEAR EQUATIØN)
30	READ INPUT TAPE 7,5,F,E,G,P,Q,D,DT
35	WRITE ØUTPUT TAPE 6,40,N,IMAX,F,E,G,P,Q,D,DT
40	FØRMAT(15HOPRØBLEM NUMBER I2/I4/7E14.6)
50	T(1)=0.0
85	V(1)=0.0
45	DØ 120 I=1,IMAX
55	T(I+1) = T(I)+DT
56	IF(F*T(I)-50.)57,57,59
57	Z(I)=(.02*EXPF(F*T(I))-.02)/(EXPF(F*T(I+1))+P)
58	GØ TØ 60
59	Z(I)=.02
60	IF(F*T(I))-25.)65,65,80
65	X1=(EXPF(F*T(I))+P)/(EXPF(F*T(I+1))+P)
70	X2=E*DT+G*LØGF(X1)
75	GØ TØ 90
80	X2=E*DT-G*F*DT
90	B=V(I)+X2
95	Y=V(I)+X2-Q*DT*(SQRTF(B)*B**3.0-SQRTF(V(I))*V(I)**3.0)/(B-V(I))
100	IF(ABSF(Y-B)-D)115,115,105
105	B=Y
110	GØ TØ 95
115	V(I+1)=Y
120	CØNTINUE
125	WRITE ØUTPUT TAPE 6,130
130	FORMAT(112HO T Z V T Z V T Z V)
(continuation)	
135	J1=1
140	J2=3

Table 10. (Continued)

STATEMENT NUMBER	FORTRAN STATEMENT
145	WRITE ØUTPUT TAPE 6,150,(T(I),Z(I),V(I),I=J1,J2)
150	FØRMAT(1H 9E13.6)
155	J1=J1+3
160	J2=J2+3
165	IF(IMAX+3-J2)170,170,145
170	GØ TØ 15

Table 11. Sample input for IBM-704 program: Solutions to Kristianson Nonlinear Equation

PROBLEM: $S = 10^{13}$, $x = 20$

1 150	Card 1
1.8046E-06 8.0391E-09 4.8753E-04 9.6257E-01 2.0455E-04 1.E-06	Card 2
1.E+05	Card 3

XV. APPENDIX D: LIST OF SYMBOLS

Table 12. List of symbols used in text

SYMBOL	MEANING
a	$(\alpha - \alpha \ln \alpha + \frac{1}{2}\alpha(\ln \alpha)^2 - 1)/(1 - \alpha)$
a'	constant in equation 124
c	specific heat
d	mass density
f	function
g	number of secondary atoms produced by a primary atom
i	subscript denoting the ith point
j	subscript denoting the jth iteration
k	Boltzmann constant
n	neutron density
n'	constant in equation 125
p	probability that a neutron will be transferred from one given energy to another given energy in one collision
p'	constant in equation 125
q	neutron slowing down density
r	radial distance
$\underline{r}$	position vector
r_T	maximum radius of a spherical thermal spike at which the temperature exceeds the melting temperature of niobium
s	$x_1 - x_2 - 1$
t	time
u	neutron lethargy
v	neutron velocity

Table 12. (Continued)

SYMBOL	MEANING
x	rectangular coordinate
x_1	T_1'/Q_d
x_2	T_2'/Q_d
y	E_o/E
z_n	$(\alpha^{1/(1-\alpha)} \ln \alpha^n y)/(1-\alpha)$
A	atomic weight
A'	constant of integration
A''	constant of integration
A_m	number of atoms whose temperature exceeds the melting temperature of niobium in a given thermal spike
$\bar{A}_m$	average number of atoms whose temperature exceeds the melting temperature of niobium in the average spike in a given set of thermal spikes
A_n	$\sum_{m=0}^{n-1}{}' (m-n)^m \theta^m/m!$
C	constant of integration
C'	constant of integration
C_{1-6}	rate constants
$C_n(E)$	Placzek correction factor in the nth interval
$\overline{C_n(E)}$	average of $C_n(E)$ in the nth interval
D	diffusion coefficient
E	neutron energy
E_o	source neutron energy
E_u	upper neutron energy
F	constant of integration

Table 12. (Continued)

SYMBOL	MEANING
F_{as}	$\Sigma_s \phi$, the total asymptotic collision density
F_n	collision density in the nth interval
F_p	defined by equation 85
F_s	scattering collision density
F_1	defined by equation 123a
F_2	defined by equation 123b
G	cross section for atomic displacement
I	ratio of interstitial atoms to regular lattice positions
$J_n(z)$	$\sum_{m=0}^{n} J_{n-m}(0)\ (-z)^m/m!$
K_n	$E\ F_n$
N	atomic density
N(E)	defined by equations 79 and 99
$N_s(E)$	defined by equation 88a
P_{is}	probability that a moving atom will not be lost in a sink (other than a vacancy)
P_{iv}	probability that a moving atom will not combine with an existing vacancy
P_{vi}	probability that an existing vacancy will not be filled by a moving atom
P_{vs}	probability that an existing vacancy will not be lost in a sink (other than an interstitial)
Q	energy initially imparted to a thermal spike
Q_d	energy imparted to a thermal spike which is less than the displacement energy
R_{ai}	fractional temperature annealing rate for interstitials

Table 12. (Continued)

SYMBOL	MEANING
R_{av}	fractional temperature annealing rate for vacancies
R_{pi}	fractional production rate for interstitials
R_{pv}	fractional production rate for vacancies
R_{ri}	fractional radiation annealing rate for interstitials
R_{rv}	fractional radiation annealing rate for vacancies
S	fission neutron source strength
S_{norm}	normalized fission neutron source strength
S_p	defined by equation 86
S_t	defined by equation 87
T	absolute temperature
T'	energy of a moving atom
T_m	maximum attainable energy of a displaced atom
$T(\tau)$	time part of the slowing down density with the variables separated
T_1'	energy of the primary atom
T_2'	energy of the secondary atom
V	ratio of vacant lattice positions to regular lattice positions
$X(x)$	spatial part of the slowing down density with the variables separated
α	$(A - 1)^2/(A + 1)^2$
γ	a/ξ
γ_{1-8}	orders of reaction
δ	Dirac delta function
δ'	convergence criterion

Table 12. (Continued)

SYMBOL	MEANING
ϵ_I	interstitial activation energy
ϵ_V	vacancy activation energy
ζ	$1 + (\alpha \ln \alpha)/(1 - \alpha)$
θ	$\alpha^{1/(1-\alpha)} \ln (\alpha^{-1/(1-\alpha)})$
λ_s	scattering mean free path for neutrons
$\bar{\mu}_o$	$2/3A$
σ	microscopic cross section
σ_a	microscopic absorption cross section
σ_s	microscopic scattering cross section
τ	Fermi age
ϕ	neutron flux
ϕ_{as}	asymptotic neutron flux
Λ	$(dT/d\tau)(1/T)$
Σ	macroscopic cross section
Σ_a	macroscopic absorption cross section
Σ_s	macroscopic scattering cross section