Influence of a Variable Ejection Probability on the Displacement of Atoms

ALVIN E. FEIN
Westinghouse Research Laboratories, Pittsburgh, Pennsylvania

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A model for the displacement of atoms is used in which each atom of a crystal has a threshold energy that is a random variable. Three quantities are derived as a function of the probability density of this random variable. First the total number of displaced lattice atoms resulting from an initial energetic atom is found as a function of the kinetic energy of the moving atom. Second, the average number of displaced lattice atoms per atom initially displaced by external radiation is derived. Third, the total number of displaced atoms resulting from a given dose of radiation is determined. Both charged particle and neutron radiation are considered. It is shown that the shapes of all these quantities, for moderately large energies of the bombarding particles, are independent of the nature of the probability density governing the displacement energy; the probability density determines only an amplitude factor. It is shown further that the physical effects of bombardment by either neutrons or charged particles can be pictured as arising from an "effective sharp-threshold energy" determined by the probability density functions and that this effective threshold is the same for both types of bombardment. Finally, it is shown that, if the present factor of about five between the theory of radiation damage and the corresponding experiments is to be explained solely on the basis of a variable probability of ejection, a considerable fraction of the atoms in a solid must have a surprisingly large threshold energy.

1. INTRODUCTION

ONE of the main effects of bombarding a solid with energetic particles is the displacement of the atoms in the solid. The problem of determining the number of such displaced atoms has received considerable theoretical study during the last few years. The understanding of this problem is important in determining the changes in physical properties of the solid, for the variations of these properties is directly dependent upon the number of displaced atoms.

In most of these investigations a model has been chosen in which the atoms in a lattice have a sharp threshold energy E_d for displacement. That is, if a lattice atom receives an energy greater than E_d, it is displaced; whereas, if it receives an energy less than E_d, it remains at its site and dissipates the acquired energy in lattice vibrations. This model is, of course, not a true picture of the situation; but it has been used because it is simple and accurate enough for qualitative discussions. However, theoretical calculations of the number of displaced atoms based on this model have been consistently in disagreement with experimental results. The theory predicts a displacement yield of five to seven times the observed amount.

There are several possible explanations for this discrepancy. One possibility is that the interpretation of the experimental measurements is in error. Thus, the relation between, say, change in resistance and number of interstitial-vacancy pairs may be inaccurate, or the effect of annealing may be much larger than assumed. However, the possibility exists that the theoretical model of radiation damage is inadequate. In this paper we shall be concerned with the possibility that error is introduced in the theoretical calculation of the number of displaced atoms by the assumption of a sharp threshold.

It is natural to suppose that the displacement threshold energy will not be sharp, but there will be, for any energy E, some probability that a lattice atom which gains that energy will be displaced. There are several reasons why the threshold energy is not sharp. One such reason is that the energy required to free an atom will depend upon the crystallographic direction of the initial velocity of the atom as it starts to leave its site.[1] Another is that the state of the thermal vibration in the neighborhood of the struck atom will influence the amount of energy necessary to dislodge the atom. Further, during the collision process energy may be lost by acoustic radiation.

A few workers have studied models in which the threshold energy for displacement is not sharp. Sampson, Hurwitz, and Clancy[2] (SHC) have used an ejection probability defined as follows. An atom receiving an energy E has a probability $P(E)$ of escaping, where

$$P(E)=\begin{cases}0, & E\leq E_0\\ (E-E_0)/(E_1-E_0), & E_0\leq E\leq E_1\\ 1, & E\leq E_1.\end{cases}\quad(1.1)$$

On this model of the displacement threshold they have calculated approximately, as a function of x, the total number, $g(x)$, of displaced atoms which are produced by an initial displaced atom of kinetic energy x.

Snyder and Neufeld[3] have also considered a nonsharp threshold. Further, they have also considered the possibility that, in a collision between two atoms, the originally stationary atom will be displaced, while the incident atom replaces it in the lattice. They perform a calculation in which (1.1) is taken as the probability of ejection, and $1-P(E)$ as the probability of replacement.

In what follows we shall calculate the total number of displaced atoms both for the case of an initial knock-on lattice atom and for two types of incident primary

[1] W. L. Brown and W. M. Augustyniak, Bull. Am. Phys. Soc. Ser. II, 2, 156 (1957).
[2] Sampson, Hurwitz, and Clancy, Phys. Rev. 99, 1657 (1955).
[3] W. S. Snyder and J. Neufeld, Phys. Rev. 103, 862 (1956).

radiation. Our calculations will be similar to those of SHC in that the possibility of replacement will not be considered. It will, however, be more general in the model chosen for the threshold and more accurate in the method used for solving the equations. The object of our more refined treatment was to discover whether the above-mentioned discrepancy between theoretical and experimental results could arise solely from the broadness of the threshold.

In Sec. 2 we derive a general prescription for the determination of the function $g(x)$ mentioned above, valid for any dependence of ejection probability on energy. In Sec. 3 we consider certain special forms of the ejection probability.

In Secs. 4 and 5 we calculate $\bar{\nu}(T_m)$, the total number of displaced atoms per primary displaced atom, where the primary is displaced by some incident bombarding particle capable of transferring, in a single collision, a maximum energy T_m. Knowing this function we then derive the total number, $D(K)$, of displaced atoms resulting from a given flux of incident radiation of energy K. Section 4 deals with charged particles as the incident radiation, Sec. 5 with neutrons.

We have obtained two principal results of a general nature. The first is that the shape of $D(K)$, for moderately large values of K, regardless of the type of radiation, is unaffected by the extent or form of the ejection probability; these properties of the probability determine only a scale factor in $D(K)$. Further this scale factor is shown to be the same for both neutron bombardment and charged particle bombardment. Thus a given material behaves exactly as if there existed some "effective sharp-threshold energy," regardless of the type of radiation, as long as K is sufficiently large.

The second result is that, if the inclusion of a variable ejection probability is to explain the present discrepancy between theory and experiment, one must have a large range of energies over which $P(E)$ is neither zero nor one. That is, there need be a considerable fraction of the lattice atoms which require a liberating energy many times the minimum threshold energy E_0.

2. GENERAL FORMALISM

We wish to determine the total number of atoms in a solid which are displaced as the result of giving to a single lattice atom a certain amount of kinetic energy. We assume that an atom receiving an energy E below some energy E_0 will never escape and that there exists an energy E_1 sufficiently large to liberate any atom with certainty. We assume further that a given stationary lattice atom has a threshold energy E_d which is a random variable with a range from E_0 to E_1. Quantitatively, the probability that an atom has a threshold energy between E_d and E_d+dE_d is given by $f(E_d)dE_d$. The probability density function (p.d.f.) $f(E_d)$ has the properties

$$f(E_d)=0 \quad \text{if} \quad E_d<E_0 \quad \text{or} \quad E_d>E_1, \tag{2.1}$$

and

$$\int_{E_0}^{E_1} f(E_d)dE_d=1. \tag{2.2}$$

We shall henceforth measure energies in units of E_0. In particular

$$E_1=aE_0, \tag{2.3}$$

$$E_d=yE_0, \tag{2.4}$$

$$E=xE_0, \tag{2.5}$$

so that Eqs. (2.1) and (2.2) read, respectively,

$$f(y)=0 \quad \text{if} \quad y<1 \quad \text{or} \quad y>a, \tag{2.6}$$

$$\int_1^a f(y)dy=1. \tag{2.7}$$

Let $g(x)$ be the total number of displaced lattice atoms resulting from a moving atom of the solid with kinetic energy x. (The original atom is included in this total.) In considering the interaction between the atoms of the solid, we shall assume hard-sphere collisions. That is, in a collision between a moving atom of kinetic energy x and a stationary atom, it is equally likely that any amount of energy between 0 and x is transferred.

We formulate the equations in the same manner as that in which Seitz and Koehler[4] treat the problem of a sharp threshold. Consider the collision between an atom of kinetic energy x (denoted by A) and a stationary atom (denoted by B). The total number of displacements produced by the initial atom will equal the sum of the individual totals produced by A and B after the collision. If an energy u is transferred, after the collision A will have energy $x-u$ and B will have energy $u-y$ (if the threshold energy of B is y). Under the hard-sphere collision assumption the probability of transferring an energy between u and $u+du$ is du/x. Thus

$$g(x)=\int_0^x \frac{du}{x}g(x-u)+\int_0^\infty dyf(y)\int_0^x \frac{du}{x}g(u-y). \tag{2.8}$$

In the above, the integration over y results from the fact that the energy necessary to displace the atom is not known but follows the p.d.f. $f(y)$. Differentiating (2.8)

$$dg/dx=(1/x)\int_0^\infty f(y)g(x-y)dy. \tag{2.9}$$

We then wish to solve the above under the condition

$$g(x)=0 \quad \text{if} \quad x<0, \tag{2.10}$$

$$g(x)=1 \quad \text{if} \quad 0\leq x\leq 1. \tag{2.11}$$

[4] F. Seitz and J. S. Koehler, *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1956), Vol. 2, pp. 381 ff.

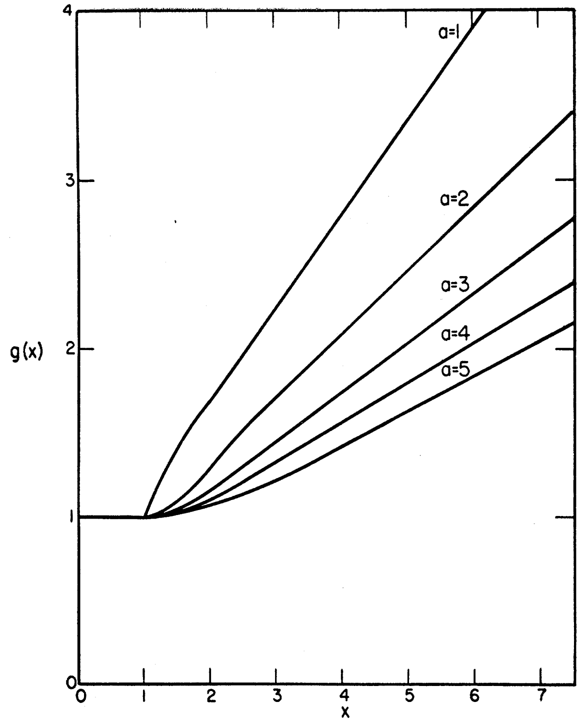

FIG. 1. Number of displacements, $g(x)$, per primary displaced atom of energy x for several values of the parameter a.

A formal solution to (2.9) can be found through the use of the Laplace transform. This is done in the Appendix, the solution, Eq. (A12), being

$$g(x)=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\frac{e^{sx}}{s}\exp\left\{\int_s^\infty dzF(z)/z\right\} \quad \text{for } \sigma>0, \tag{2.12}$$

where $F(s)$ is the Laplace transform of $f(x)$,

$$F(s)=\int_0^\infty e^{-sx}f(x)dx. \tag{2.13}$$

It is shown further in the Appendix that, for large values of x, the function of (2.12) reaches an asymptotic curve

$$g(x)\underset{x\gg1}{\longrightarrow}A(x+B), \tag{2.14}$$

where

$$A=e^{-\gamma}\exp(-\langle\ln x\rangle_{\text{Av}}), \tag{2.15}$$

$$\langle\ln x\rangle_{\text{Av}}=\int_1^a dxf(x)\ln x, \tag{2.16}$$

$$B=\langle x\rangle_{\text{Av}}=\int_1^a dxxf(x), \tag{2.17}$$

and γ is Euler's constant: $\gamma=0.577$.

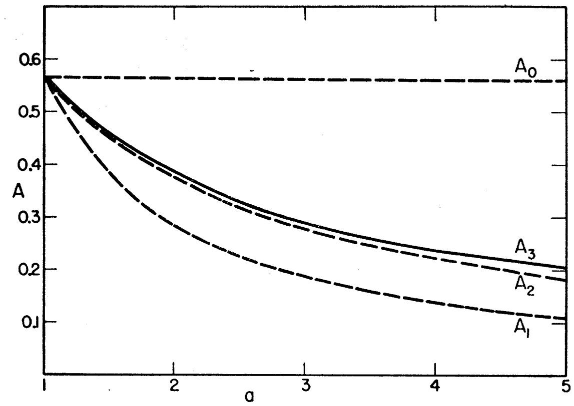

FIG. 2. Amplitude factor, A, as a function of the width a of the p.d.f. for several forms of the p.d.f.

For small values of x, Eq. (2.9) must be solved piecewise in x. Consider the region $1>x>2$. The solution to (2.9) in this region can be found by using the known value of $g(x)$ in the region $0>x>1$. Thus, for $1>x>2$,

$$\begin{aligned} g(x)&=1+\int_1^x\frac{dz}{z}\int_1^z dyf(y) && \text{if } x>a \\ &=1+\ln(x/a)+\int_1^a\frac{dz}{z}\int_1^z dyf(y) && \text{if } x<a. \end{aligned} \tag{2.18}$$

Numerical calculations were made for selected values of $f(x)$. It was found that, for values of a at least up to $a=5$ and for any p.d.f., the function $g(x)$ could be very well represented by (2.14) for $x\geq2$. We then have our function $g(x)$ for all x by (2.10), (2.11), (2.18), and (2.14).

From (2.14) it can be seen that, irrespective of the p.d.f., the asymptotic form of $g(x)$ will always be linear, the slope of the line depending upon the distribution through (2.15). Secondly, from (2.17) we have always

$$B\leq a, \tag{2.19}$$

so that for large values of x, one can neglect the additive term in (2.14) again irrespective of the p.d.f.

3. ILLUSTRATION OF THE METHOD FOR SPECIAL CASES

Let us take as an example

$$\begin{aligned} f_3(x)&=1/(a-1), && 1\geq x\geq a \\ &=0 && \text{otherwise.} \end{aligned} \tag{3.1}$$

This is the example treated by SHC. We note in the limit $a\rightarrow1$ we reach the case of a sharp threshold.

Now for the case of (3.1)

$$\langle \ln x\rangle_{\mathrm{Av}}=-1+\frac{a\ln a}{a-1}, \tag{3.2}$$

$$A_3=e^{1-\gamma}\exp\left\{-\frac{a\ln a}{a-1}\right\}=1.511\exp\left\{-\frac{a\ln a}{a-1}\right\}, \tag{3.3}$$

$$B_3=\tfrac{1}{2}(a+1). \tag{3.4}$$

Figure 1 shows plots of $g(x)$ *vs* x for various values of a for the case of (3.1). We compare this case to the three limiting cases

$$f_0(x)=\delta(x-1), \tag{3.5}$$

$$f_1(x)=\delta(x-a), \tag{3.6}$$

$$f_2(x)=\delta[x-\tfrac{1}{2}(a+1)], \tag{3.7}$$

for which

$$A_0=e^{-\gamma}=0.561, \tag{3.8}$$

$$B_0=1, \tag{3.9}$$

$$A_1=e^{-\gamma}/a=0.561/a, \tag{3.10}$$

$$B_1=a, \tag{3.11}$$

$$A_2=2e^{-\gamma}/(a+1)=1.122/(a+1), \tag{3.12}$$

$$B_2=\tfrac{1}{2}(a+1). \tag{3.13}$$

In Fig. 2 we plot A_0, A_1, A_2, and A_3 as functions of a. As shall be shown below in Secs. 4 and 5, the quantity A is directly proportional to the total number of displacements resulting from a source of radiation of fixed energy. The curves of A_0, A_1, and A_3 are essentially the curves presented by SHC. They make the qualitative observation that a system governed by the p.d.f. $f_3(x)$ appears to behave more strongly like one having a threshold at $x=a$ than one having a threshold at $x=1$. This conclusion can be seen more directly from (3.2) which shows that, for the p.d.f. $f_3(x)$, $\langle \ln x\rangle_{\mathrm{Av}}$ is closer to $(1/a)$ than it is to zero. Even more accurate would be the statement that such a system behaves more as one having a threshold at $x=(a+1)/2$, i.e., a threshold at the midpoint of the range of $f_3(x)$. This result is an approximation of the more general statement of (4.21) below.

4. BOMBARDMENT BY CHARGED PARTICLES

In the preceding we have been concerned with the number of lattice atoms which are displaced, *given* an initial atom of kinetic energy x. In a physical situation, however, it is only the external source of radiation which is known. It is thus necessary to be able to calculate the number of atoms of the solid which are displaced as a function of the type and energy of the incident radiation. By use of the results of Sec. 2, this can be easily done if the kinetic energy distribution of the lattice atoms displaced by the incident radiation is known.

Let the bombarding particles have a mass M_1 and a kinetic energy K, and let the mass of the stationary lattice atoms be M_2. Further let

$$T_m=\frac{4M_1M_2}{(M_1+M_2)^2}K \tag{4.1}$$

be the maximum possible total energy transfer between one of the bombarding particles and a stationary atom in the solid during one collision. Denote the total energy transfer in a given collision by T.

We shall now determine the total number of displaced atoms in the solid per primary displaced atom. We denote this quantity by $\bar{\nu}$. By defining the problem in this manner, one need not be concerned at present with the subject of cross sections.

We shall first treat the case in which the encounter is governed by a Coulomb force so that one has Rutherford scattering, i.e., the probability of an energy transfer between T and $T+dT$ is proportional to dT/T^2. This type of reaction governs most cases in which a beam of charged particles is incident on a solid. Denoting this case by a subscript R, we have

$$\bar{\nu}_R(T_m,a)=\mu_R(T_m,a)/\psi_R(T_m,a), \tag{4.2}$$

where

$$\mu_R(T_m,a)=\int_0^{T_m}dyf(y)\int_y^{T_m}\frac{dT}{T^2}g(T-y), \tag{4.3}$$

$$\psi_R(T_m,a)=\int_0^{T_m}dyf(y)\int_y^{T_m}\frac{dT}{T^2}. \tag{4.4}$$

To evaluate the above integrals it is necessary to know the relative values of T_m and a. It is also necessary to know whether or not a is greater than two. Since we are primarily interested in values of T_m at least several times the maximum threshold energy, we restrict the following discussion to the case

$$T_m>a+2. \tag{4.5}$$

From (4.4) for all values of a satisfying (4.5)

$$\psi_R(T_m,a)=-(1/T_m)+\int_1^a\frac{dy}{y}f(y)$$
$$=\langle 1/y\rangle_{\mathrm{Av}}-(1/T_m). \tag{4.6}$$

The evaluation of $\mu_R(T_m,a)$ is fairly long although straightforward. The results can be written

$$\mu_R(T_m,a)=C_R(a)+A\ln T_m, \tag{4.7}$$

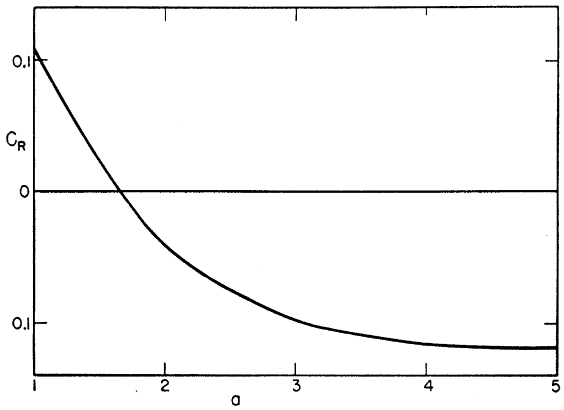

FIG. 3. The values of C_R as a function of a for the p.d.f. $f_3(x)$.

where A is given in (2.15); for $1 \leq a \leq 2$

$$C_R(a) = -A + \int_1^a dy f(y) \times \left\{ \frac{1+\ln(2/a)+\ln(a+y)-\ln(2+y)}{y} + \frac{2A+AB-1+\ln(a/2)}{y+2} - A\ln(y+2) + \frac{2-a}{(y+a)(y+2)} \int_1^a \frac{dz}{z} \int_1^z f(u)du + \int_1^a \frac{dx}{(x+y)^2} \int_1^x \frac{dz}{z} \int_1^z f(u)du \right\}, \quad (4.8a)$$

and for $a \geq 2$

$$C_R(a) = -A + \int_1^a dy f(y) \left\{ \frac{1}{y} - \frac{1-AB-2A}{y+2} - A\ln(y+2) + \int_1^2 \frac{dx}{(x+y)^2} \int_1^x \frac{dz}{z} \int_1^z f(u)du \right\}. \quad (4.8b)$$

Thus (4.2) can be written

$$\bar{\nu}_R(T_m,a) = \frac{C_R + A\ln T_m}{\langle 1/y\rangle_{\text{Av}} - (1/T_m)}. \quad (4.9)$$

In general C_R is small so that one can neglect the additive constant in (4.7) for large T_m. [The values of $C_R(a)$ for the case of (3.1) are shown in Fig. 3.] Thus the shape and range of the p.d.f. is manifest only in the "amplitude factor" A. For this case of large T_m we can then write (4.9) as

$$\bar{\nu}_R(T_m,a) = \frac{A}{\langle 1/y\rangle_{\text{Av}}} \ln T_m. \quad (4.10)$$

We shall now derive the total number, $D_R(K)$, of displaced atoms resulting from a bombardment by a beam of charged particles of time integrated flux ϕ and initial energy K. [The relation between T_m and K is given by (4.1).] If n_0 is the density of atoms in the solid, $\sigma_d(k)$ the cross section for displacement by a charged particle of kinetic energy k, S the area bombarded, and

$$t_m = \frac{4M_1M_2}{(M_1+M_2)^2}k, \quad (4.11)$$

then the number of atoms which are displaced as the energy of the charged particle drops from k to $k-dk$ as it moves a distance dr through the solid is given by

$$dD_R = Sn_0\phi\sigma_d(k)\bar{\nu}_R(t_m)dr, \quad (4.12)$$

so that, if K_f is the final energy of the bombarding particle as it leaves the material ($K_f=0$ if the particle does not emerge),

$$D_R(K) = Sn_0\phi \int_{K_f}^K dk\,|dk/dr|^{-1}\sigma_d(k)\bar{\nu}_R(t_m). \quad (4.13)$$

The expression (dk/dr) is the rate of energy loss of the charged particle as it passes through the solid. Its value is well-known empirically.

From the theory of Coulomb scattering we have for the differential cross section for transfer of an energy t

$$d\sigma = (G/k)dt/t^2, \quad (4.14)$$

where, with e being the charge of an electron, Z_1 and Z_2, respectively, the charge of the bombarding particle and the atomic number of the atoms in the solid, and E_0 the minimum threshold mentioned in Secs. 1 and 2,

$$G = \frac{\pi Z_1^2 Z_2^2 e^4 M_1}{E_0^2 M_2}. \quad (4.15)$$

(The quantity E_0 appears above because it was chosen as our unit of energy.) Thus

$$\sigma_d(k) = (G/k)\int_1^a f(y)dy \int_y^{t_m} dt/t^2 = (G/k)[\langle 1/y\rangle_{\text{Av}} - (1/t_m)], \quad (4.16)$$

which for large t_m becomes

$$\sigma_d(k) = (G/k)\langle 1/y\rangle_{\text{Av}}. \quad (4.17)$$

Now there exists some value, K_0, such that for $k > K_0$, one can use (4.17) to represent $\sigma_d(k)$ and t_m is sufficiently large to justify replacing $\bar{\nu}_R(t_m)$ by the form given in (4.10). In general, experimental conditions are such that

$$K \gg K_0. \quad (4.18)$$

If also we have $K_f > K_0$, i.e., a thin target, then the limiting forms for $\bar{\nu}_R(t_m)$ and $\sigma_d(k)$ can be used in (4.13) for the entire range of integration, and (4.13) becomes

$$D_R(K)=n_0\phi GAS\int_{K_f}^{K}dk|dk/dr|^{-1}\frac{\ln t_m}{k}. \tag{4.19}$$

If on the other hand the target is thick (i.e., $K_f \ll K_0$) one can with good accuracy simply replace the lower limit of (4.19) by K_0 since the effects produced by the charged particles along the small length of path where its energy is so low can be neglected. Then for $K_f \ll K_0$ we can write

$$D_R(K)=n_0GAS\int_{K_0}^{K}dk|dk/dr|^{-1}\frac{\ln t_m}{k}. \tag{4.20}$$

From (4.19) and (4.20) we obtain directly the result that the only influence of the p.d.f. on the value of $D_R(K)$ arises through the multiplication factor A. Thus comparing the general form (2.15) to the cases of sharp thresholds, (3.8) and (3.10), one sees that for large values of the energy, K, of the bombarding particle the number of resultant displacements, $D_R(K)$, is identical to that which would result if the solid exhibited a sharp threshold at $x=c$. This "effective sharp-threshold energy" c is given by

$$c=\exp(\langle\ln x\rangle_{\text{Av}}). \tag{4.21}$$

5. BOMBARDMENT BY NEUTRONS

Let us now consider the case in which the bombarding particles are neutrons, denoted by a subscript N. We shall assume that the neutron-atom interaction is of the hard-sphere type, an assumption which proves to be a fair approximation. Thus in analogy to (4.2)

$$\bar{\nu}_N=\mu_N(T_m,a)/\psi_N(T_m,a), \tag{5.1}$$

where

$$\mu_N(T_m,a)=\int_0^{T_m}dyf(y)\int_y^{T_m}dTg(T-y), \tag{5.2}$$

and

$$\psi_N(T_m,a)=\int_0^{T_m}dyf(y)\int_y^{T_m}dT. \tag{5.3}$$

Again take $T_m>a+2$. Then (5.3) becomes immediately

$$\psi_N(T_m,a)=T_m-B, \tag{5.4}$$

and (5.2) reads

$$\mu_N(T_m,a)=\tfrac{1}{2}AT_m^2+C_N, \tag{5.5}$$

where, if $a\geq 2$

$$C_N=2-A(2+2B+B^2)+(A/2)\int_1^a f(y)y^2dy+\int_1^2 dx\int_1^x(dz/z)\int_1^z f(u)du, \tag{5.6a}$$

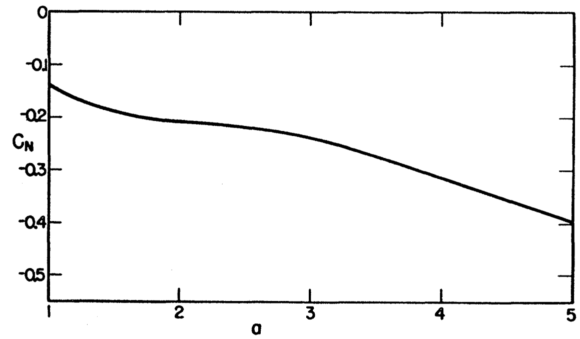

FIG. 4. The values of C_N as a function of a for the p.d.f. $f_3(x)$.

and if $a\leq 2$

$$C_N=2-A(2+2B+B^2)+2\ln(2/a)+(A/2)\int_1^a f(y)y^2dy+(2-a)\int_1^a(dz/z)\int_1^z f(u)du+\int_1^a dx\int_1^x(dz/z)\int_1^z f(u)du. \tag{5.6b}$$

The form $\bar{\nu}_N$ can be written

$$\bar{\nu}_N(T_m,a)=\frac{\tfrac{1}{2}AT_m^2+C_N}{T_m-B}. \tag{5.7}$$

As in the case of Rutherford scattering, the additive constant C_N is small. [Figure 4 shows a plot of $C_N(a)$ for the case in which the p.d.f. is $f_3(x)$.] Thus for large T_m

$$\bar{\nu}_N(T,a)=\tfrac{1}{2}AT_m. \tag{5.8}$$

We note that for Rutherford scattering $\bar{\nu}_R$ went as $\ln T_m$; whereas in the case of neutron bombardment $\bar{\nu}_N$ is linear in T_m.

We now wish to find $D_N(K)$, the total number of displacements resulting from a bombardment by a beam of neutrons with an energy K. Since the neutron cross section for elastic scattering $\sigma_s(K)$ is so small, it is very unlikely that a given neutron will undergo more than one collision during its passage through a sample. Thus the expression for $D_N(K)$ is derived much more simply than the corresponding expression for charged particles. With n_0 and ϕ as defined in the last section, we have directly, V being the volume irradiated

$$D_N(K)=Vn_0\phi\sigma_s(K)\bar{\nu}_N(T_m). \tag{5.9}$$

Then for values of K sufficiently large so that $\bar{\nu}_N(T_m)$ can be written as in (5.8) the above becomes

$$D_N(K)=Vn_0\phi A\sigma_s(K)T_m/2. \tag{5.10}$$

Therefore as in the charged-particle case, the p.d.f. enters only in the amplitude factor A so that under neutron bombardment also the solid behaves as if it has a sharp threshold at $x=c$.

6. CONCLUSIONS

At present the simple theory of sharp threshold energy is used to treat the displacement of lattice atoms by incident radiation. In almost all cases this theory predicts a number of displacements from five to seven times that which is actually observed experimentally. If one attempts to explain this discrepancy solely by the introduction of a variable probability of ejection with the p.d.f. $f_3(x)$, the above discussions, especially Fig. 2 and Eq. (2.15), would require one to suppose that there are atoms in the solid needing energies of about ten times the minimum threshold energy in order to be displaced. This figure seems considerably higher than one would estimate intuitively. Since there are as yet no experimental data sufficiently accurate to give much insight into the form of the p.d.f. governing the displacement of lattice atoms, we have used the distribution $f_3(x)$ to arrive at this conclusion. Of course, changing the p.d.f. would alter its necessary range somewhat, but not significantly. Thus perhaps the discrepancy (if the error is solely in the theoretical calculation of $\bar{\nu}$) is due to some other effects. One such possibility is the nature of the collision between lattice atoms. If, instead of hard sphere collisions, one hypothesized a mechanism which favored transference of small energies, the value of $\bar{\nu}$ would be further reduced.

Also we have shown that, for moderately large values of the energy of the bombarding particles, a solid behaves as if there existed some sharp-threshold energy governing the displacements of the lattice atoms. Further the solid exhibits the same effective sharp threshold both for neutron and charged particle bombardment. Thus to detect the presence of a broad threshold it would be necessary to use incident particles of fairly low energies. However, because of the relations (4.9) and (5.7) one need not use values of T_m only slightly greater than the minimum threshold to detect the presence of broad threshold as usually stated. In fact one can employ a considerable range of the energies of the bombarding particles before the difference between (4.9) and (4.10) or (5.7) and (5.8) become indistinguishable. Experiments in this energy range would yield some information about the p.d.f. although one would not be able to determine it completely.

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APPENDIX

We seek the solution to (2.9). That equation can be written

$$x\frac{dg}{dx}=\int_0^x f(y)g(x-y)dy. \quad \text{(A1)}$$

In the above, by dint of (2.10) we have replaced the upper limit, ∞, of (2.9) by x.

Taking the Laplace transform of (A1) gives

$$-\frac{d}{ds}[sG(s)-g(0+)]=F(s)G(s), \quad \text{(A2)}$$

where $G(s)$ is the Laplace transform of $g(x)$ and $F(s)$ the Laplace transform of $f(x)$. The value of $g(0+)$ is given by (2.11) as

$$g(0+)=1. \quad \text{(A3)}$$

Equation (A2) can be written

$$\frac{d}{ds}(sG)=-\left(\frac{F(s)}{s}\right)(sG), \quad \text{(A4)}$$

so that

$$\ln(sG)=\ln C+\int_s^\infty \frac{F(z)}{z}dz, \quad \text{(A5)}$$

where

$$C=\lim_{s\to\infty}(sG). \quad \text{(A6)}$$

Therefore

$$G(s)=\frac{C}{s}\exp\left\{\int_s^\infty \frac{F(z)}{z}dz\right\}, \quad \text{(A7)}$$

and

$$g(x)=\frac{C}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\frac{e^{xs}}{s}\exp\left\{\int_s^\infty \frac{F(z)}{z}dz\right\} \quad (\sigma>0). \quad \text{(A8)}$$

We must evaluate the constant C. By the definition of Laplace transform, Eq. (A6), and Eq. (2.11)

$$C=\lim_{s\to\infty}s\left[\int_0^1 e^{-sx}dx+\int_1^\infty e^{-sx}g(x)dx\right]$$

$$=\lim_{s\to\infty}s\left[-\frac{1}{s}(e^{-s}-1)+\int_1^\infty e^{-sx}g(x)dx\right]=1. \quad \text{(A9)}$$

Then finally

$$g(x)=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} ds\frac{e^{xs}}{s}\exp\left\{\int_s^\infty \frac{F(z)}{z}dz\right\} \quad (\sigma>0). \quad \text{(A10)}$$

The above equation can be put into a more useful form by noting some of the properties of $F(s)$. Since $F(s)$ is the Laplace transform of $f(x)$ we have

$$F(s)=\int_0^\infty e^{-sx}f(x)dx. \quad \text{(A11)}$$

Therefore

$$\int_s^\infty \frac{F(z)}{z}dz=\int_s^\infty dz\int_0^\infty dx\frac{e^{-zx}}{z}f(x). \quad \text{(A12)}$$

Integrating first with respect to z, we have

$$\int_s^\infty \frac{F(z)}{z}dx=\int_0^\infty dxf(x)J(s,x), \qquad \text{(A13)}$$

where

$$J(s,x)=\int_s^\infty \frac{e^{-zx}}{z}dz. \qquad \text{(A14)}$$

Integrating $J(s,x)$ by parts, we obtain

$$J(s,x)=-e^{-sx}\ln s+x\int_s^\infty dxe^{-zx}\ln z. \qquad \text{(A15)}$$

Let

$$K(s,x)=J(s,x)+\ln s. \qquad \text{(A16)}$$

Then

$$K(0,x)=\lim_{s\to 0}[1-e^{-sx}]\ln s+x\int_0^\infty dxe^{-zx}\ln z$$
$$=-(\gamma+\ln x). \qquad \text{(A17)}$$

In the above the limit term goes to zero, and the integral can be evaluated by the theory of gamma functions; γ is Euler's constant, $\gamma=0.577$. From (A16) and (A14),

$$\frac{\partial K(y,x)}{\partial y}=\frac{1}{y}-\frac{e^{-yx}}{y}=-\sum_{j=1}^{\infty}(-1)^j x^j\frac{y^{j-1}}{j!}. \qquad \text{(A18)}$$

Integrating both sides of (A18) from $y=0$ to $y=s$, we get

$$K(s,x)=K(0,x)-\sum_{j=1}^{\infty}(-1)^j\frac{(xs)^j}{jj!}. \qquad \text{(A19)}$$

Then, from (A17) and (A16), the above reduces to

$$J(s,x)=-\ln s-\gamma-\ln x-\sum_{j=1}^{\infty}(-1)^j\frac{(xs)^j}{jj!}. \qquad \text{(A20)}$$

We recall that $f(x)$ is a probability density with the properties given in (2.6) and (2.7). Thus, if (A20) is inserted into (A13), we get

$$\int_s^\infty \frac{F(z)}{z}dx=-\ln s-\gamma-\langle \ln x\rangle_{\text{Av}}$$
$$+s\langle x\rangle_{\text{Av}}-\sum_{j=2}^{\infty}(-1)^j\frac{s^j\langle x^j\rangle_{\text{Av}}}{jj!}, \qquad \text{(A21)}$$

where we have written out explicitly the first term of the summation, and $\langle \ln x\rangle_{\text{Av}}$ and $\langle x^j\rangle_{\text{Av}}$ are the average values of $\ln x$ and x^j, respectively:

$$\langle \ln x\rangle_{\text{Av}}=\int_0^\infty dxf(x)\ln x, \qquad \text{(A22)}$$

$$\langle x^j\rangle_{\text{Av}}=\int_0^\infty dxf(x)x^j. \qquad \text{(A23)}$$

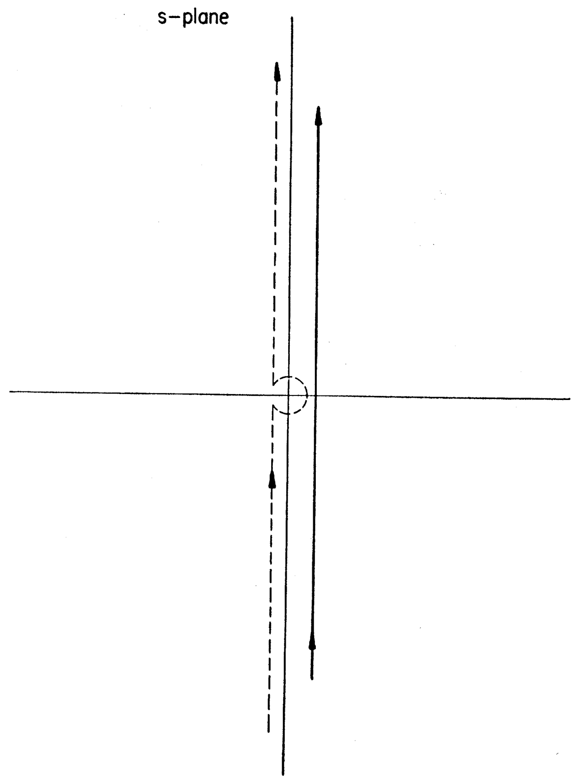

FIG. 5. Paths of integration for Eq. (A24).

We can put the expression of (A21) into (A10) to obtain

$$g(x)=\frac{e^{-\gamma}e^{-\ln x}}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{\exp[s(x+\langle x\rangle_{\text{Av}})]}{s^2}$$
$$\times\exp\left\{-\sum_{j=2}^{\infty}(-1)^j\frac{s^j\langle x^j\rangle_{\text{Av}}}{jj!}\right\},\quad \sigma>0. \qquad \text{(A24)}$$

The contour for the above is the solid line shown in Fig. 5.

If we wish to obtain the asymptotic value of $g(x)$ as x becomes very large, we can simply move the contour slightly to the left of the imaginary axis so that $\text{Re}\{s\}<0$, evading the pole at $s=0$ as shown. Then, with x large, we can ignore the contribution of the integral over all the path except for the circuit about $s=0$. At $s=0$, the integrand of (A24) has a pole of second order. Thus

$$g(x)\underset{x\to\infty}{\longrightarrow} e^{-\gamma}\exp(-\langle \ln x\rangle_{\text{Av}})$$
$$\times\frac{\partial}{\partial s}\left[\exp[s(x+\langle x\rangle_{\text{Av}})]\exp\left\{-\sum_{j=2}^{\infty}(-1)^j\frac{s^j\langle x^j\rangle_{\text{Av}}}{jj!}\right\}\right]_{s=0}$$
$$=[e^{-\gamma}\exp(-\langle \ln x\rangle_{\text{Av}})](x+\langle x\rangle_{\text{Av}}). \qquad \text{(A25)}$$