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NEUTRON DAMAGE IN GRAPHITE

HUBERT M. JAMES
Purdue University

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PHYSICS DIVISION

NEUTRON DAMAGE IN GRAPHITE

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This report gives an analysis of the damage produced by fast neutrons in graphite crystals. The end results are

(a) estimates of the energy stored in the crystal, in displaced carbon atoms, per neutron of a given initial energy, and

(b) estimates of the relative damage produced by the neutron distributions existing at several points in a pile.

SEC. I. INTRODUCTION

In this report no attempt is made to extend earlier calculations of the cross-sections for the primary processes which occur when an energetic particle traverses a graphite crystal. The values for the energy loss in inelastic collisions (electronic excitation) by recoiling carbon atoms traversing the crystal are taken from the report by Brown[1]. The discussion of elastic collisions is based on formulas derived by application of the Born approximation and the statistical model of the atom. The derivation of these formulas is given in some detail by Seitz[2]; the same formulas are given by Brown[1] in a different notation.

The present report does go beyond the earlier discussion of Seitz in its detailed analysis of the cumulative effects of these processes. The treatment of Seitz is based on the observation that energy losses in elastic collisions increase rapidly as the energy of the particle decreases, whereas energy losses by inelastic collisions decrease rapidly. There is therefore a rather narrow energy range in which the two processes involve comparable losses. Seitz therefore assumes that one can get a satisfactory approximation by neglecting elastic collisions completely when the inelastic collisions are dominant, and neglecting inelastic collisions completely when elastic collisions are dominant. This assumption simplifies the analytical developments of the theory, and it is certainly justified in the first approximation. It will be shown later, however, that the somewhat extreme point of view implicit in this approximation may be misleading in some respects. Its avoidance in the present treatment has required considerable use of graphical calculations, and the presentation of the principal results in graphical rather than analytical form.

The present treatment differs from that of Seitz also in the greater detail in the division of the elastic collisions into those producing thermal agitation of the crystal, slow secondaries (knocked-on atoms) and fast secondaries. Finally, the calculations are carried to new and concrete end results.

A valuable aid for concrete thinking about such problems is the reduction of collision cross-sections and rates of energy loss to terms of "probability of a collision per layer of atoms traversed" and "average energy loss per layer of

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atoms traversed." These quantities will be defined, not in terms of the actual crystal structure of the crystal, but in terms of a simple cubic lattice of equal density. Let the spacing of the atoms in such a crystal be

$$d = N^{-1/3}, \tag{1}$$

where N is the number of atoms per unit volume. We define the "geometrical cross-section" of an atom in this crystal as

$$A = d^2 . \tag{2}$$

If σ is the collision cross-section for a given type of collision, the probability of such a collision per unit length of path in the crystal is σ/d^3, and the "probability of a collision per crystal layer traversed" is

$$p = d \cdot \frac{\sigma}{d^3} = \frac{\sigma}{A} . \tag{3}$$

The "energy loss per layer" is defined as

$$H = d \cdot \frac{dE}{dx} . \tag{4}$$

In graphite, $d \simeq 2.1\ \text{Å} \simeq a_H$.

SEC. II. ENERGY LOSSES IN INELASTIC COLLISIONS

Following Brown[1], we estimate this energy loss in inelastic collisions of carbon atoms traversing graphite by multiplying the observed losses of carbon atoms in air by a factor 1635, representing the difference in densities of the materials, and a factor due to the different scattering cross-sections for carbon atoms and "air atoms." The latter factor, ranging from 0.97 for the lowest energies, to 0.94 for the highest, is extrapolated from observations quoted by Brown. The results are given in Table I. The first two columns give the velocity and energy of the ions, and the last two the rates of energy loss per centimeter and per layer (H_i). The method of estimation is certainly unreliable at the lowest energies, where the energy transferred in a collision becomes comparable to the differences in energy of a valence electron in the gas and in the solid, or to the electronic band widths in the crystal.

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TABLE I

RATES OF ENERGY LOSS BY CARBON ATOMS MOVING THROUGH GRAPHITE. INELASTIC COLLISIONS ONLY.

$V \times 10^{-8}$ (cm/sec)	E (ev)	$\left(\frac{dE}{dx}\right)_I$ (mev/cm)	H_i (ev/layer)
0.5	5,230	524	10.8
1	20,900	1,350	27.8
2	83,700	3,900	80.5
3	184,200	7,650	157
4	335,000	11,500	237
5	523,000	13,800	284
6	753,000	15,150	312
7	1,030,000	15,400	317
8	1,340,000	15,500	219

SEC. III. ELASTIC COLLISIONS

The formulas given by Brown and by Seitz for the transfer of energy in elastic collisions between atoms can be reduced to the following form.

Let the incident particle have mass M_1, atomic number Z_1, energy E_1, and the (originally stationary) scattering atom mass M_2, atomic number Z_2. Then the cross-section for a collision involving transfer of energy greater than ϵ is (for $\epsilon < \delta E$)

$$\delta = M_1 Z_1^2 \cdot 4\pi a_H^2 \frac{Z_2^2}{M_2} \frac{E_R}{E_1 + E} \frac{E_R}{E_1\delta + \epsilon} \left[1 - \frac{\epsilon}{E\delta}\right] , \tag{5}$$

where

E = Ionization energy of hydrogen atom = 13.54 ev,

a_H = Bohr radius,

$$\delta = \frac{4M_1M_2}{(M_1 + M_2)^2} , \tag{6}$$

$$E_1 = \frac{0.229}{8} \cdot \{ Z_1^{1/3} + Z_2^{1/3} \} \cdot \frac{m}{M^2} \cdot E_R , \tag{7}$$

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m being the electronic mass.

In what follows σ will always be expressed as a multiple of the geometrical cross-section A, so that it becomes numerically equal to the probability p of collision per layer, and energies will always be expressed in volts. It will be convenient to write

$$\sigma(e) = \Gamma \cdot \frac{1}{E_1 + E} \cdot \frac{1}{E_1\delta + \epsilon} \cdot \left[1 - \frac{\epsilon}{E\delta}\right] , \tag{8}$$

where

$$\Gamma = \frac{M_1}{M_2} Z_1^2 Z_2^2 \cdot \frac{4\pi a_H^2}{A} \cdot E_R^2 \tag{9}$$

is a constant with the dimensions of energy-squared.

The values of the constants for the problem at hand are given in Table II. For a light fission fragment (LFF) we have taken $M_1 = 95$, $Z_1 = 38$; for a heavy fission fragment (HFF), $M_1 = 139$, $Z_1 = 54$.

TABLE II

VALUES OF CONSTANTS IN ELASTIC SCATTERING FORMULA

	C in Graphite	LFF in Graphite	HFF in Graphite
$\Gamma\left(\frac{ev^2}{A}\right)$	1.96×10^5	6.20×10^7	1.84×10^7
E_1 (ev.)	0.00185	0.00943	0.0151
δ	1.	0.399	0.293

The following derived formulas may be noted.

The probability that an incident atom with energy E will transfer to a lattice atom an energy ϵ to within $d\epsilon$ is

$$d\sigma = \frac{\Gamma d\epsilon}{E(E_1\delta + \epsilon)^2} , \qquad \epsilon < \delta E ,$$
$$d\sigma = 0 , \qquad \epsilon > \delta E . \tag{10}$$

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The average energy transfer to the crystal, per layer traversed, in processes involving transfer of energy greater than ϵ_m is

$$H_e(\epsilon_m) = \int_{\epsilon_m}^{\delta E} \epsilon \frac{d\sigma}{d\epsilon} \epsilon$$

$$= \frac{\Gamma}{E} \left\{ \ln \left(\frac{\delta E + \delta E_1}{\epsilon_m + \delta E_1} \right) + \frac{\delta E_1}{\delta E + \delta E_1} - \frac{\delta E_1}{\epsilon_m + \delta E_1} \right\} \qquad (11)$$

The following approximate forms are useful:

$$H_e(\epsilon_m) \simeq \frac{\Gamma}{E} \ln \left(\frac{\delta E}{\epsilon_m} \right) \quad , \text{ if} \qquad \delta E,\ \epsilon_m \gg \delta E_1 \qquad (12)$$

$$H_e(0) = H_e \simeq \frac{\Gamma}{E} \left[\ln \left(\frac{E}{E_1} \right) - 1 \right] \quad , \text{ if} \qquad E \gg E_1 \qquad (13)$$

SEC. IV. PRELIMINARY DISCUSSION OF ELASTIC COLLISIONS

Collision Producing Heat

When a particle passing through a crystal undergoes an elastic collision with one of the atoms of the lattice, it may knock this atom from its position in the lattice and cause a more or less permanent change in the structure of the crystal.

If the lattice atom acquires only a small amount of energy in the collision (distant collision) it will be set into vibration, but will not be able to leave its cell in the crystal. Most of its vibrational energy will very quickly be shared with neighboring atoms; the energy transferred to the crystal by the colliding particle is harmlessly dissipated in heat.

In other collisions a lattice atom may acquire so much energy that it is driven far away through the crystal, coming to rest in an interstitial position, and leaving behind a more or less permanent hole.

When a lattice atom acquires enough energy to remove it to an interstitial position, but not a great deal more than the required amount, it may or may not leave its position, depending on the circumstances of the collision. Its energy may be quickly shared with other atoms and converted into heat. Or the struck atom may be moved only to an adjacent interstitial position. Re-

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arrangement of one or two other atoms in the lattice will then fill the original hole, allow the displaced atom to fall into a lattice position, and thus restore the perfection of the crystal lattice with all the energy transferred in the collision transformed into heat. The greater the energy acquired in the collision, the farther will the struck atom move through the lattice, and the smaller will be the probability that such a "healing" process will occur during a given period of observation.

We now define the energy ϵ_t such that the number of collisions producing displaced atoms is equal to the number of collisions in which the energy transfer exceeds ϵ_t. A collision with energy transfer ϵ_t will actually have about an even chance of producing a permanently displaced atom. We shall, however, treat all energy transfers greater than ϵ_t as leading to displaced atoms, and all transfers of less energy as resulting only in the production of heat. The quantity ϵ_t thus plays a very important role in the analysis which is to follow.

For purposes of calculation we shall take $\epsilon_t = 25$ ev. It will be evident from the discussion above that this does not represent the minimum energy required to displace an atom, or the energy stored in the crystal per displaced atom, but a quantity which may be several times as large. Even in a very favorable collision resulting in a permanently displaced atom a good deal of energy will be wasted in heat.

Residual Energy

Let us now consider a very energetic charged particle moving through the graphite lattice. The probability that it will knock an atom out of a given layer will be given by Eq. (7), with $\epsilon = \epsilon_t$. Since $E_1\delta \ll \epsilon_t \leqslant \delta E$, one will have with good approximation

$$\sigma(\epsilon_t) = \Gamma/E\epsilon_t \tag{14}$$

A very energetic particle will leave behind widely-spaced displaced atoms, but as its energy decreases these will occur closer and closer together. When $\sigma(\epsilon_t) = 1$, (that is, when on the average there is a displaced atom per layer) the trail of displaced atoms will be essentially continuous. Indeed, some of the displaced atoms will in turn have enough energy to displace other atoms, and a very high probability of displacing such atoms from the very next layer. Thus when the energy of the particle has been reduced to about

$$E_c = \Gamma/\epsilon_t \tag{15}$$

by elastic and inelastic collisions, this residual energy will very quickly be

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dissipated in a series of elastic collisions which produce an essentially continuous damaged region in the crystal. One finds for

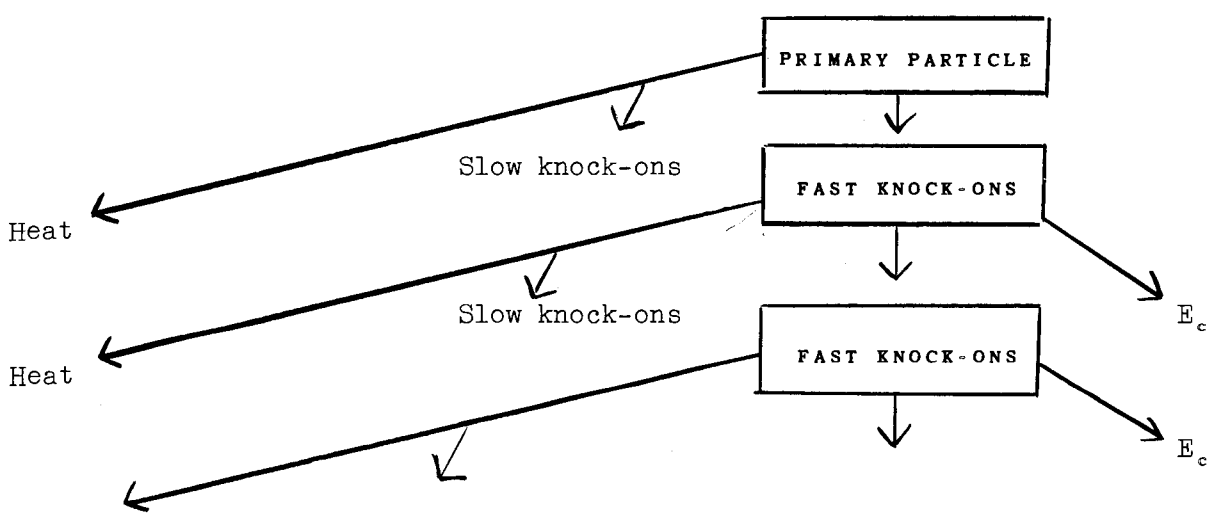
carbon atoms in graphite,	$E_c = 7850$ ev.
LFF in graphite,	$E_c = 2.47 \times 10^6$ ev.
HFF in graphite,	$E_c = 7.36 \times 10^6$ ev.

Slow and Fast Knock-Ons

The energy E_c computed for a lattice atom passing through the lattice (here, carbon passing through graphite) marks a second important division in the range of energy transfers ϵ. A knocked-on atom with energy ϵ, where $\epsilon_t < \epsilon < E_c$, will be called a slow knock-on. It may have only enough energy to reach a nearby interstitial position, producing a single vacant lattice space, or it may have enough energy to knock on other lattice atoms, producing a single continuous damaged region, as described above.

A knocked-on atom with energy $\epsilon > E_c$ will be called a fast knock-on. The dissipation of its energy in producing heat, slow knock-ons, and even fast knock-ons, can be discussed as though it were a primary particle.

The dissipation of the energy of a primary particle can then be described by the following diagram.



The primary particle (fission fragment or neutron) produces heat, slow knock-ons, and fast knock-ons, until its energy is dissipated. The fast knock-ons in turn produce heat, slow knock-ons, and fast knock-ons, until their energy is reduced to the "residual" value E_c expended in producing a continuous damaged region. This new generation of fast knock-ons dissipates its energy in the same way, and so on.

The energy of the primary particle ultimately appears as heat, the energy of the slow knock-ons, and the residual energies E_c of fast knock-ons. How much of this energy is quickly dissipated as heat, and how much is stored in the crystal as lattice imperfections, will be discussed in Section VI.

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Low Energy Cut-Off

Equation (8) gives a finite total cross section,

$$\sigma(0) = \Gamma/E_1\delta(E_1 + E) \quad , \tag{16}$$

for all collisions, however small the transfer of energy. For small E, however, this total cross section becomes very large. For instance, if $E = E_c$ one has

$$\sigma(0) = \frac{\Gamma}{E_1\delta(E_1 + E_c)} \cong \frac{\Gamma}{E_1\delta E_c} = \frac{\epsilon_t}{E_1\delta} \tag{17}$$

For carbon knock-ons in graphite this is about 13,500 : that is, the formula indicates that there are some 13,500 collisions involving transfer of energy per layer traversed by the carbon atom! Of course the vast majority of these collisions involve a very small transfer of energy; they represent "collisions" with lattice atoms in the layer that are quite distant from the point where the carbon atom passes through.

Equation (8) is based on the consideration of a collision between two isolated atoms. It might reasonably be applied in treating the collision of a fast particle with the lattice atoms nearest the point where it passes through a crystal layer, but its application to the collision of two atoms separated by many intervening atoms seems to be quite unjustified. One would anticipate that the reaction of the intervening atoms would prevent energy transfers directly to the more distant atoms. In using this formula one is therefore led to consider the possibility of applying a cutoff, neglecting all collisions with a collision parameter above a given value, or all energy transfers below a given value.

What type of cutoff should be used is an interesting fundamental problem that can not be considered here. It is evident that any cutoff of the low-energy, heat-producing collisions will increase the fraction of the energy going into high-energy processes which produce lattice damage. The possible importance of this factor has been explored by introducing a low-energy cutoff limiting the total cross section to a definite multiple of A, nA. The minimum energy transfer considered, ϵ_m, then depends on the energy E of the fast particle. If $\delta E_1 \ll \epsilon_m \ll E\delta$, one has, by Eq. (8),

$$n = \sigma(\epsilon_m) \cong \Gamma/E\epsilon_m \tag{18}$$

or

$$\epsilon_m \cong \Gamma/nE \tag{19}$$

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The condition for the validity of this approximation may be written as

$$(\Gamma/n\delta)^{1/2} \quad << \quad E \quad << \quad \Gamma/n\delta E_1 \tag{20}$$

and is satisfied for all reasonable choices of n and $E > E_c$.

In the calculations with cutoff to be presented later, n has been chosen to be 5, as representing a probable minimum value. The introduction of this low energy cutoff changes the results of the calculation appreciably, but not radically.

SEC. V. METHOD OF CALCULATION

Here there will be indicated very briefly the methods employed in the calculations on which the later discussion is based.

The cross section for energy losses ϵ such that $\epsilon_1 \leqslant \epsilon \leqslant \epsilon_2$ is obviously

$$\Delta\sigma = \sigma(\epsilon_1) - \sigma(\epsilon_2) \quad . \tag{21}$$

We define special cross sections, for layer traversed, as follows.

σ_1 :	for $0 \leqslant \epsilon \leqslant \epsilon_t$.	Heat-producing collisions without low-energy cutoff.
σ_1' :	for $\epsilon_m \leqslant \epsilon \leqslant \epsilon_t$.	Heat-producing collisions with low-energy cutoff.
σ_2 :	for $\epsilon_t \leqslant \epsilon \leqslant E_c$.	Collisions producing slow knock-ons.
σ_3 :	for $E_c \leqslant \epsilon$.	Collisions producing fast knock-ons.

One can obtain simple formulas for all these quantities by introducing into Eq. (8) approximations appropriate to the values of E, ϵ_1 and ϵ_2 under consideration.

$$\sigma_1 \cong \epsilon_t E_c/\delta E_1 E \tag{22a}$$

$$\sigma_1' \cong n - E_c/E \quad , \qquad E\delta >> \epsilon_t \tag{22b}$$

$$\sigma_2 \cong E_c/E \quad , \qquad E\delta >> \epsilon_t \tag{22c}$$

$$\sigma_3 \cong \epsilon_t/E\ (1 - E_c/\delta E), \qquad E\delta > E_c \tag{22d}$$

The energy loss per layer, in elastic collisions with $\epsilon_1 \leqslant \epsilon \leqslant \epsilon_2$, is

$$\Delta H_e = H_e(\epsilon_1) - H_e(\epsilon_2) \tag{23}$$

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We define the energy losses per layer traversed, H_1, H_1', H_2, H_3, corresponding to the cross sections σ_1, σ_1', σ_2, σ_3, respectively. Then, by Eqs. (12) and (13), we have for all $\delta E > E_c$:

$$H_1 \cong \epsilon_t E_c/E \quad ln(\epsilon_t/\delta e E_1) \quad , \tag{24a}$$

$$H_1 \cong \epsilon_t E_c/E \quad ln(nE/E_c) \quad , \tag{24b}$$

$$H_2 \cong \epsilon_t E_c/E \quad ln(E_c/\epsilon_t) \quad , \tag{24c}$$

$$H_3 \cong \epsilon_t E_c/E \quad ln(\delta E/E_c) \quad . \tag{24d}$$

The total loss in elastic collisions, per layer, without cutoff, is

$$H_e = \epsilon_t E_c/E \quad ln(E/eE_1) \quad . \tag{25a}$$

With cutoff, the total loss becomes

$$H_e' = \epsilon_t E_c/E \quad ln(\delta n E^2/\epsilon_t E_c) \tag{25b}$$

We define also H_i, the total loss in inelastic collisions, per layer.

Let the total loss of energy per layer be H:

$$H = H_i + H_e \qquad \text{(no cutoff)} \quad , \tag{26a}$$

$$H = H_i + H_e' \qquad \text{(with cutoff)} \quad . \tag{26b}$$

A particle then loses energy dE in traversing dE/H(E) layers. As its energy decreases from E_1 to E_2 it will produce, on the average,

$$N_s = \int_{E_1}^{E_2} \frac{dE}{H(E)} \sigma_2(E) \tag{27}$$

slow secondaries having a total energy

$$H_s = \int_{E_1}^{E_2} \frac{dE}{H(E)} H_2(E) \quad . \tag{28}$$

[A more rigorous justification of these expressions is easily given.]
The amount of energy going into heat or fast secondaries, and the total number of fast secondaries can be computed similarly. Because of the rather complicated form of H(E), such integrals are often best obtained by graphical integration.

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When $H_i(E)$ is negligible, as in the case considered in the next section, analytic results are conveniently obtained.

SEC. VI. ENERGY STORED IN THE CRYSTAL

In discussing the actual damage to a crystal traversed by fast particles one needs to know how much of the energy of the knocked-on atoms is eventually stored in the crystal in the form of lattice imperfections, and how much is quickly dissipated as heat. The following discussion of this difficult problem is highly tentative, because the low-energy cutoff is not introduced, despite its evident importance for the low-energy processes under consideration. Furthermore, it is not known how much "healing" of the crystal arises from atomic rearrangements taking place soon after the disturbance occurs.

Slow Knock-ons

Since $\epsilon_t \gg E_1\delta$, it follows from Eq. (10) that the probability that a slow knock-on has an energy ϵ will vary with $1/\epsilon^2$, whatever the energy $E > E_c$, or the distribution of energies, of the primary charged particles. The average energy of the slow knock-ons from fast particles is thus

$$\bar{\epsilon} = \frac{\int_{\epsilon_t}^{E_c} \epsilon \cdot \frac{1}{\epsilon^2}\, d\epsilon}{\int_{\epsilon_t}^{E_c} \frac{1}{\epsilon^2}\, d\epsilon} \cong \epsilon_t \ln \frac{E_c}{\epsilon_t} \tag{29}$$

For slow knock-ons in graphite this is about 144 e.v.

We now compute the number of secondary knock-ons due to a knock-on of initial energy E as its energy falls to the value ϵ_t. The loss of energy in inelastic collisions by these particles will be neglected, thus limiting consideration to slow knock-ons and the fast knock-ons with $E \sim 10{,}000$ e.v. In Eq. (27) we then replace E_1 by ϵ_t, E_2 by E, $H(E)$ by $H_e(E)$, and write

$$\sigma_2(E) = \sigma(\epsilon_t) \cong E_c(E - \epsilon_t)/E^2 \quad , \tag{30}$$

avoiding the approximation of Eq. (22c). Let

$$\xi = E/eE_1 \ , \quad \xi_0 = \epsilon_t/eE_1 \ , \quad \xi_1 = E_c/eE_1 \ . \tag{31}$$

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Then, on repeated integration by parts, one obtains a convenient asymptotic expansion:

$$N_s(E) = \int_{\epsilon_t}^{E} dE \frac{E - \epsilon_t}{E \quad \epsilon_t} \frac{1}{ln(E/eE_1)} = \int_{ln\,\xi}^{ln\,\xi_0} dz \frac{e^z/\xi_0 - 1}{z} \tag{32}$$

$$= \frac{E}{\epsilon_t} \cdot \frac{1}{ln\xi} \left[1 + \frac{1!}{ln\xi} + \frac{2!}{ln^2\xi} + \ldots \right] - \frac{1}{ln\xi_0} \left[1 + \frac{1!}{ln\xi_0} + \frac{2!}{ln^2\xi_0} + \ldots \right]$$

$$- ln \left[\frac{ln\,\xi}{ln\,\xi_0} \right] .$$

In computing the energies of these secondaries one must avoid the use of Eq. (24c), valid only for $E > E_c$. Instead, one has simply

$$H_2 = H_e(\epsilon_t) = \epsilon_t E_c/E \quad ln(E/\epsilon_t) . \tag{33}$$

since $\delta = 1$ here. Then (an <u>asymptotic</u> expansion!)

$$H(E) = \int_{\epsilon_t}^{E} dE \frac{ln(E/\epsilon_t)}{ln(E/eE_1)}$$

$$= E \left\{ 1 - \frac{ln\xi_0}{ln\xi} \left[1 + \frac{1!}{ln\xi} + \frac{2!}{ln^2\xi} + \ldots \right] \right\} + \epsilon_t \left[\frac{1!}{ln\xi_0} + \frac{2!}{ln^2\xi_0} + \ldots \right] \tag{34}$$

Calculation shows that the fastest of the slow knock-ons in carbon, $E = E_c = 7850$ e.v., produce on the average 23.2 secondary knock-ons, with an average energy of 119 e.v. A knock-on with the average energy, $E = 144$ e.v., produces on the average 0.31 secondary knock-ons, with average energy 43 e.v. The fastest knock-ons use 35.2% of their energy in producing secondary knock-ons, but the knock-ons with average energy lose only 9.3% of their energy in this way.

One can easily average these results over the energy distribution of the primary slow knock-ons. The average number of secondary knock-ons per primary [redacted]

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knock-on is

$$\bar{N}_s = \frac{\int_{\epsilon_t}^{E_c} \frac{dE}{E^2} \int_{\epsilon_t}^{E} dE' \frac{E' - \epsilon_t}{E'\epsilon_t} \cdot \frac{1}{ln\ E'/eE_1}}{\int_{\epsilon_t}^{E_c} dE/E^2} \tag{34}$$

$$= \frac{E_c}{E_c - \epsilon_t} \left\{ ln \left[\frac{ln\xi_1}{ln\xi_0} \right] + \frac{1}{ln\xi_0} \left[1 - \frac{1!}{ln\xi_0} + \frac{2!}{ln^2\xi_0} - \cdots\cdots \right] \right\}$$

$$- \frac{\epsilon_t}{E_c - \epsilon_t} \left\{ N_s(E_c) + \left[1 - \frac{1}{ln\xi_1} + \frac{2!}{ln^2\xi_1} - \cdots\cdots \right] \right\} .$$

Similarly

$$\bar{H}_s = \epsilon_t \frac{E_c}{E_c - \epsilon_t} \left\{ ln \frac{E_c}{\epsilon_t} - ln\ \xi_0\ ln \left[\frac{ln\xi_1}{ln\xi_0} \right] \right\} - \frac{\epsilon_t}{E_c - \epsilon_t} H_s(E_c) . \tag{35}$$

Calculation with these formulas shows that there are 0.545 secondary knock-ons per primary knock-on, with an average energy of 47 e.v. Since a secondary knock-on with energy 50 e.v. has, by Eq. (32), a probability of only 0.045 of producing a tertiary knock-on, it is evident that second-, third-, and higher-generation knock-ons will together total about six-tenths of the number of primary knock-ons.

The energy stored in a crystal when an atom is displaced to an interstitial position is a fraction of ϵ_t which we shall here take, for purposes of estimation, as $\frac{1}{2}$. The energy stored per slow primary knock-on will then be about $\frac{1}{2} \cdot \epsilon_t\ 1.6 = 20$ e.v., if no immediate healing takes place. Comparing this with the average energy of 144 e.v. expended in producing slow knock-ons, we would conclude that about 14% of the energy expended by energetic ($E>E_c$) particles in producing slow knock-ons will be stored in the crystal. This estimate would be raised by introduction of a low-energy cutoff, and lowered by healing.

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Fast Knock-ons

As was noted in the preceding discussion, a knock-on with energy E_c will produce 23.2 secondary knock-ons with average energy 119 e.v. A secondary with this average energy will, by Eq. (32), produce on the average 0.232 tertiary knock-ons with average energy 40 e.v.; later-generation knock-ons will be negligible. The total number of displaced atoms produced by the residual energy of a fast carbon atom will thus be roughly $1 + 23.2 + 0.24 \times 23.2 = 29.8$; the stored energy will be $29.8 \times 12.5 = 370$ e.v., which is only 4.7% of the original energy E_c.

In Eq. (32), for $E \gg \epsilon_t$ the first term is very much the most important. Thus, for a moderate range of E about E_c the number of secondary knock-ons produced by a fast knock-on is nearly proportional to E, and the fraction of its energy stored in the crystal will be nearly constant, being roughly $\frac{1}{2} \ln \xi_1$. For higher energies the proportion of stored energy will decrease, principally because of the effect of inelastic collisions.

A calculation of the average energy $\bar{\epsilon}_f$ of secondary knock-ons due to a fast knock-on of energy E shows that $\bar{\epsilon}_f$ rises from some 11,400 e.v. for E = 20,000 e.v. to 18,900 e.v. for E = 500,000 e.v. (In this calculation, account was of course taken of the effect of inelastic collisions.) As a round figure, to within the accuracy of these considerations, one might expect that 4% of the energy given to fast secondary knock-ons will eventually be stored in the crystal. This is the figure assumed in the next Section.

SEC. VII. NEUTRON DAMAGE IN GRAPHITE

Discussion of neutron damage in a pile will proceed in three stages:

1) Calculation of the energy stored in the crystal due to a single knocked-on carbon atom, as a function of its energy.

2) Calculation of the stored energy per neutron collision, as a function of the energy of the neutron involved in the collision.

3) Calculation of the total stored energy due to the distribution of neutron collisions predicted for various points in a pile.

The division of the energy of an initially fast neutron between stored energy and heat will also be indicated.

Figure I shows the energy loss per layer of a carbon recoil passing through a graphite crystal. The loss in inelastic collisions is shown separately, and the losses in elastic collisions are computed with and without cutoff. It is evident that, while at high energies the loss of energy takes place primarily in inelastic collisions, elastic collisions still occur with appreciable frequency.

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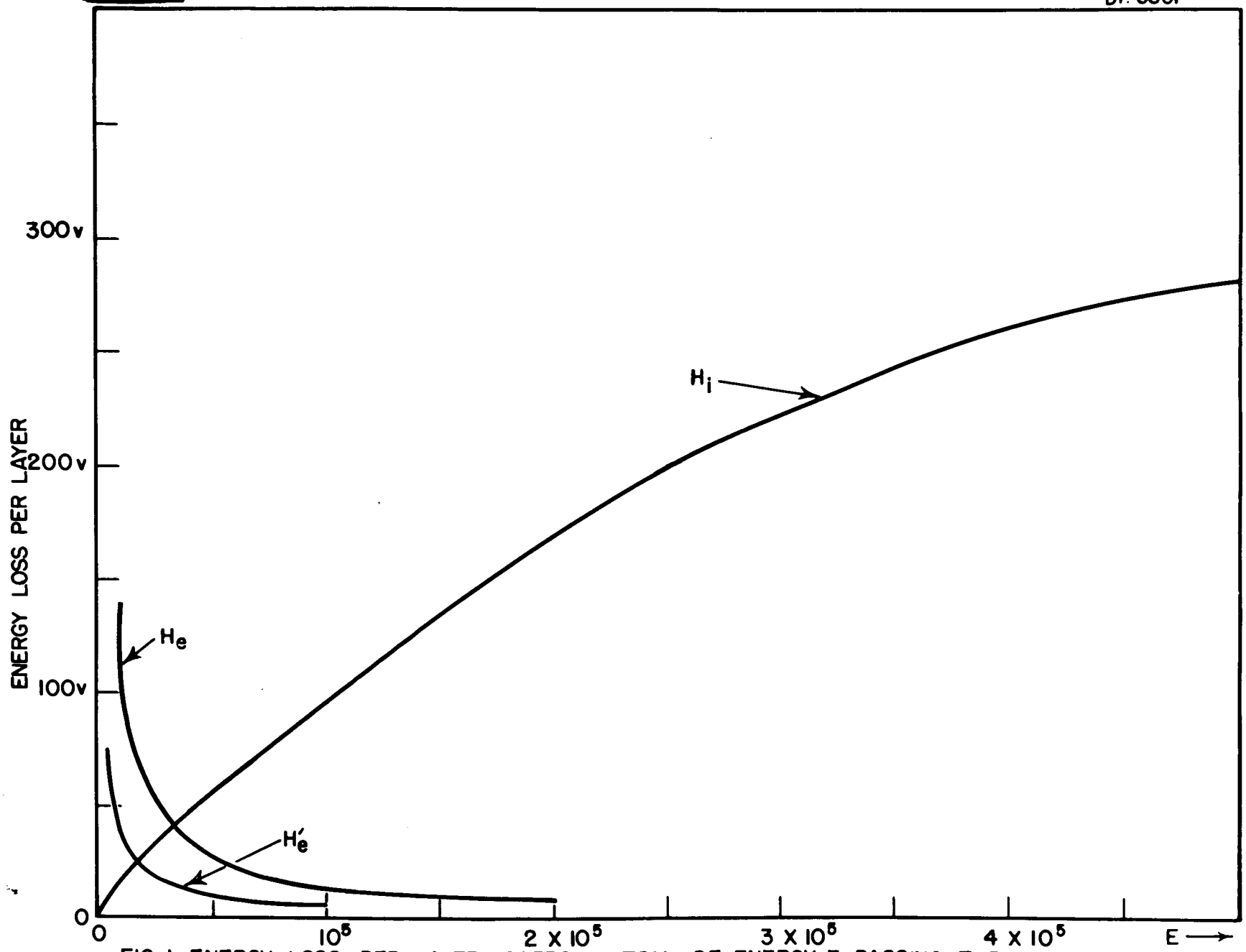

FIG. I ENERGY LOSS PER LAYER; CARBON ATOM OF ENERGY E PASSING THROUGH GRAPHITE

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Table III deals with the effects in graphite of a fast carbon atom of energy E, computed with the low-energy cutoff described in Sec. IV (cut) and without (uncut). It shows the total energy H_s of the slow knock-ons produced as the energy of the primary particle falls to E_c; the number N_f of fast knock-ons per **primary particle**; the average energy $\overline{H}_f$ of the fast knock-ons (computed for a type of cutoff intermediate between no cutoff and the kind considered here); and the total energy stored in the crystal, computed as

$$0.14\ H_s + 0.04\ N_f\overline{H}_f + 370\ \text{e.v.}$$

These terms represent the stored parts of the energy of the slow knock-ons, the energy of the fast knock-ons, and the residual energy of the original particle, respectively.

TABLE III

KNOCK-ONS IN GRAPHITE DUE TO CARBON ATOM OF ENERGY E

E (e.v.)	Energy of slow knock-ons (e.v.)		Number of fast knock-ons		Average energy of fast knock-ons (e.v.)	Stored energy (e.v.)	
	Uncut	Cut	Uncut	Cut		Uncut	Cut
10^4	270	1000				410	510
2×10^4	1700	4100	0.039	0.087	11,400	610	984
4×10^4	3600	7200	0.198	0.343	13,100	978	1560
6×10^4	4720	8640	0.302	0.476	14,300	1200	1850
8×10^4	5430	9480	0.374	0.560	15,200	1360	2040
10^5	5920	10030	0.435	0.627	15,700	1470	2170
1.5×10^5	6700	10830	0.513	0.709	16,700	1650	2360
2×10^5	7130	11270	0.574	0.751	17,300	1760	2470
3×10^5	7600	11750	0.625	0.802	18,200	1890	2600
5×10^5	8050	12200	0.676	0.851	18,900	2010	2720

The most striking result of this calculation is the slow increase in the stored energy as the energy of the primary carbon atom is increased; a tenfold increase in E from 5×10^4 e.v. to 5×10^5 e.v. scarcely doubles the stored energy.

This table makes it possible to analyze the loss of energy by a fast particle in different parts of its range, by taking differences in consecutive lines. For instance, during the time that the energy of a carbon atom falls from 5×10^5 e.v. to 3×10^5 e.v. it produces slow knock-ons with a total energy averaging 450 e.v. (uncut), and has a probability of only about 0.051 of producing a fast

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knock-on; on the average only 120 e.v. of the 200,000 e.v. energy loss will be stored in this crystal. In this sense, the energy losses in inelastic collisions will be completely dominant. On the other hand, the accumulated effect of the elastic collisions at high energies is important; a major fraction of the damage done to the crystal by an energetic particle is done at energies so high that the inelastic collisions far outweigh the elastic ones.

It will be noted that the change in stored energy due to the low-energy cutoff is almost constant for energetic particles. The low-energy elastic collisions involved in the cutoff are quite negligible so long as losses in inelastic collisions are dominant; they affect only the estimate of the damage done by the particle at the very end of its range.

Conversely, it is evident that a change in the assumed inelastic losses at low energies, such as might be due to the special structure of the crystal, will not change the estimate of stored energy by a large factor, since the energy loss in low-energy elastic collisions is dominant in this range. Even radical assumptions, such as that all energy losses for $E < 40,000$ e.v. take place in inelastic collisions, would only change the estimate of stored energy by a factor of 2. It therefore appears to the writer that Seitz (loc.cit.) has somewhat overestimated the difference in neutron damage to be expected in insulators and conductors.

The carbon atoms discussed above may be carbon atoms knocked on by energetic neutrons. Neutrons of energy E in collisions with carbon will produce knocked-on atoms with all energies from zero to 0.284 E. If one considers only s-wave scattering (as we shall here) these knocked-on atoms will have all energies in this range with equal probability. <u>The average energy stored in the crystal per neutron collision</u> can then be obtained as the numerical average of the stored energies per carbon atom, taken over the range of carbon-atom energies from 0 to 0.284 E. The results of this calculation are presented in Fig. 2.

It is of interest to see how much of the original energy of a fast neutron will eventually be stored in the crystal, as a result of all the collisions it undergoes. On the average, the neutron will lose a fraction 0.142 of its energy per collision. It will thus undergo one collision for each range of $0.0665 = -\log_{10}(1-0.142)$ in $\log_{10} E$. On plotting the energy lost per collision against $\log_{10} E$, and summing areas under the curve, one finds as the total stored energy per neutron of energy E the values shown in Fig. 3.

As to magnitude, the results given above should be regarded as no more than careful order-of-magnitude estimates, subject to serious uncertainties due to the unknown degree of "healing". The qualitative features of these curves should, however, be fairly reliable, and so should the following estimate of the relative neutron damage at several points in a pile.

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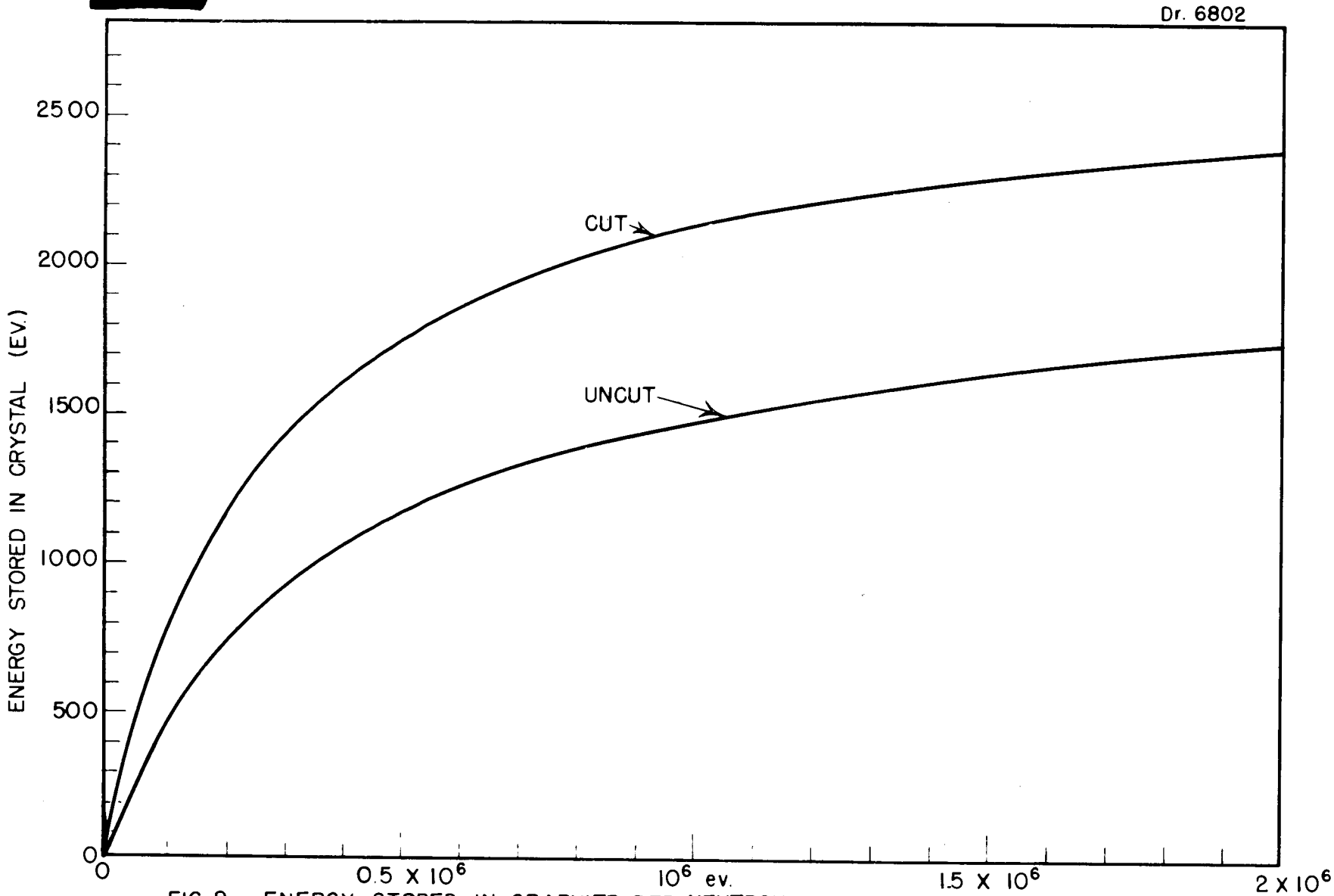

FIG. 2 ENERGY STORED IN GRAPHITE PER NEUTRON COLLISION WITH ENERGY E.

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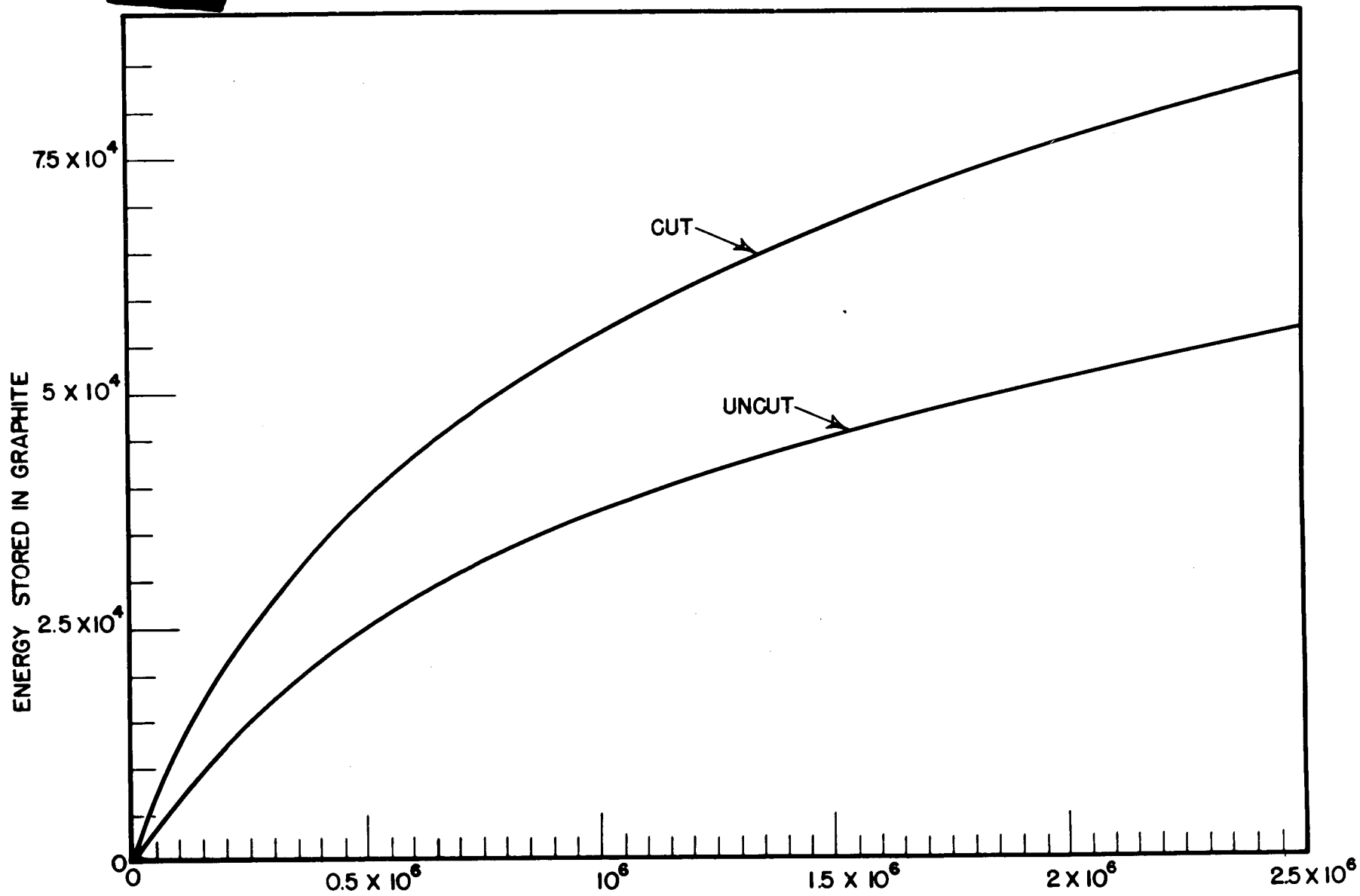

FIG. 3 PART OF NEUTRON ENERGY E EVENTUALLY STORED IN GRAPHITE

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Our estimation of neutron damage in a pile is based on the calculation of Weinberg, Stephenson and Goldberger [3] on a particular pile arrangement. They compute the flux density of neutrons, per unit range in $ln E$, for a source giving 2.347 neutrons/cm. sec. On multiplying this by $\sigma(E)$ and integrating over a given range of $ln E$, one obtains the number of collisions per atom per second, within this range of neutron energies. If the integrand contains as an additional factor the energy stored per collision, the summation yields the energy stored per atom per second. The results of graphical evaluation of these integrals are shown in Tables IV and V, which give the number of collisions and the energy stored for several ranges of E. Since almost all damage to the crystal is due to neutrons with energy greater than 10^4 e.v., the total stored energy is essentially the total for the range > 10^4 e.v., as given in Table V.

TABLE IV

$10^{24}\times$ Collisions per atom per second for a Source (Cf. Weinberg, et.al.) Giving 2.347 neutrons/cm. sec.			
	$10^4<E<10^5$	$10^5<E<10^6$	$10^6<E$
Surface of Slug	0.97	1.29	0.62
Center of Lattice	0.88	0.63	0.17

TABLE V

$10^{22}\times$ Stored Energy (e.v.) per atom per second for a Source Giving 2.347 neutrons/cm. sec.				
	$10^4<E<10^5$	$10^5<E<10^6$	$10^6<E$	Total
NO CUTOFF				
Surface of Slug	1.8	12.7	10.4	24.9
Center of Lattice	1.5	5.5	3.0	10.0
WITH CUTOFF				
Surface of Slug	3.7	19.4	14.5	37.6
Center of Lattice	3.1	8.7	4.4	16.2

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Calculations have been made of the rate of storage of energy at the surface of the slug, and in the center of the lattice. The effect of the low-energy cutoff is most marked in the treatment of the low energy collisions, and for the center of the lattice, where the low energy collisions are more important. The estimated stored energy is increased 50 to 60% by the introduction of cutoff, and, in addition, may be radically modified by healing. On the other hand, the rate of storage of energy at the two points, which is 2.49 without cutoff, is reduced only to 2.32 by the introduction of cutoff. There is little reason to expect the degree of healing to vary much from one point to the other. Thus one can conclude, as perhaps the most secure result of these considerations, that the ratio of neutron damage at the surface of the slug to that at the center of the lattice considered by Weinberg is about 2.4.

The writer is indebted to Dr. Sidney Siegel for the calculation of the results given in Table III.

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(2) Seitz, F., and Allen, A. O., "Irradiation Physics," M-4075.

(3) Weinberg, A.M., Stephenson, J., and Goldberger, N., "Neutron Flux in W Lattice," CP-G-2439, November 30, 1944.

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