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CALCULATION OF RADIATION DAMAGE EFFECTS OF
800-MeV PROTONS IN A "THIN" COPPER TARGET

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ABSTRACT

Radiation damage effects of 800-MeV protons incident on a 1-cm-thick copper target have been calculated by using the nucleon-meson transport code to determine the nuclear reactions produced by the protons, and the theory of Lindhard *et al.* to evaluate the resultant damage energy deposited in the target. Damage effects were found to be uniform across the 1-cm target thickness, and the results obtained can be expressed in cross-section form applicable to target thicknesses from about 0.01 cm to 2 cm. The calculation yielded a damage energy cross section (depending somewhat on beam and target geometry) of about 350 barn-keV and a nuclear transmutation cross section of 1.0 barn, and indicated copious proton, neutron, and helium production. Comparison of the cross sections obtained with those of several neutron spectra of reactor interest suggests that medium-energy proton bombardment may be a useful method for simulating neutron-induced radiation damage effects.

I. INTRODUCTION

A calculation has been made of the damage effects produced by 800-MeV protons incident on a copper target thin enough (≤ 1 cm) so that damage effects are uniformly distributed in depth, but thick enough so that most charged secondaries stop within the target. The Nucleon-Meson Transport Code¹ (NMTC) developed at Oak Ridge National Laboratory, in a version somewhat modified by Seeger² at Los Alamos Scientific Laboratory, was used to determine the numbers and kinetic energies of the spallation nuclei and of the light nuclei and neutrons produced in the series of nuclear interactions initiated by the incident protons. In order to estimate the lattice damage due to the energetic charged particles so produced, the corresponding damage energy (resultant kinetic energy of lattice nuclei)

was calculated using the theory of Lindhard and co-workers.³⁻⁵ The damage energy cross section due to the neutrons produced was obtained by utilizing a code developed for this purpose by Parkin and Goland.⁶ Results from this code also permit one to determine the approximate number of neutrons with a given energy spectrum required to produce the "same" amount of damage (in the damage energy sense) as an 800-MeV proton.

Damage energy is deposited in the target by the spallation and light nuclei and by the neutrons produced by the proton bombardment. A damage energy cross section describing the effect of the energetic spallation and light nuclei produced by an 800-MeV proton in copper was calculated and found to be about 330 barn-keV, with the spallation nuclei contributing almost 98% of this total. The damage energy

effect of the neutrons produced by the 800-MeV proton can be stated in terms of a "qualified" damage energy cross section expressed as 39.5 barn-keV/cm times a factor depending on beam and target geometry and having units centimeters; this factor is of order 1/2 cm for uniformly irradiated targets with linear dimensions all of the order 1 cm, and scales with linear target dimensions. The total effective damage energy cross section is the sum of the damage energy cross section for the spallation and light nuclei and the appropriate geometrically weighted cross section for the neutron. The cross section for the production of spallation nuclei other than ^{63}Cu and ^{65}Cu was found to be 0.99 b, and that for ^4He 0.16 b. (The latter result may be low by a factor of two or more-- see below). Protons and neutrons are produced in copious quantities, with cross sections of 2.5 and 3.4 b, respectively. Of the kinetic energy originally given to the spallation nuclei in the nuclear reactions, about 13% is eventually deposited in the lattice as damage energy. For the light nuclei the damage efficiency is much lower, only about 0.02% of the initial kinetic energy of these particles ultimately being deposited in the lattice as damage energy.

Calculation of the nuclear reactions produced by the protons is discussed in Section II, and the determination of the damage energy due to the resulting energetic nuclei and neutrons is considered in Section III. In Section IV the correlation with neutron damage energy cross sections is given, and in Section V inferences are drawn concerning the possible advantages of neutron damage simulation by medium-energy proton irradiation.

II. NUCLEAR REACTION CALCULATIONS

As stated in the Introduction, analysis of the inelastic nuclear interactions produced by the 800-MeV protons incident on the copper target was handled by means of the Monte Carlo Nucleon-Meson Transport Code¹ developed at Oak Ridge. The current Los Alamos version of this program incorporates some modifications by Seeger² to decrease running time, update the mass table and formula, ensure energy conservation, and provide information on time dependence if desired. The code calculates the reactions produced when a primary projectile which may be a nucleon or a pion is incident on a target which may consist of a number

of different spatial regions of various shapes, each containing a variety of specified nuclides in assigned proportions. The program allows the primary particle to interact with a target nucleus in an intranuclear cascade in which scattering from individual nucleons with possible associated production of nucleons and pions occurs according to experimentally determined cross sections in energy regions where these cross sections are available, and according to certain theoretical estimates of these cross sections in regions where they are not. At the completion of the intranuclear cascade, the excited nucleus is allowed to "evaporate" light nuclei (p, n, ^2H , ^3H , ^3He , and ^4He). No light nuclei more massive than ^4He are emitted in the evaporation model used. Pions ejected from the nucleus in the intranuclear cascade phase and nucleons emitted in either the cascade or evaporation phase are transported further and allowed to have additional nuclear interactions as long as their energies remain above certain programmer-specified cutoffs. Evaporation ^2H , ^3H , ^3He , and ^4He and below-cutoff pions and nucleons are not transported further, except that stopped negative pions may be required to have nuclear interactions. Charged projectiles experience energy losses to electrons and trajectory spreading due to nuclear Coulomb scattering as they move through the target, but transfer of momentum from projectiles to target nuclei by Coulomb scattering is not included in the code. "Events" of a variety of types are recorded on tape, including nuclear interactions with or without emission of high-energy (above-cutoff) particles, particle crossings of internal or external boundaries, and slowing of a charged particle to cutoff. In a nuclear interaction event the types and kinetic energies of the spallation nucleus and the light cascade and evaporation particles and nuclei produced are determined, in addition to other data not relevant here.

Some comparisons of the predictions of the code with experimental observations have been made by Armstrong,⁷ by Armstrong and collaborators,^{8,9} and by Bertini, Guthrie, and Culkowski.¹⁰ In general, cross sections for production of spallation nuclides are reasonably good, with accuracy to a factor two or better, though there are exceptions. Production cross sections for neutrons and singly charged light nuclei appear to be correct to a factor less than

two. In a comparison of calculated alpha production by 1-GeV protons on ^{100}Ru with experimental observations of alpha production by 950-MeV protons in nuclear emulsions, however, Bertini *et al.*¹⁰ find the calculated value low by a factor of about three. Data on the accuracy of the predicted kinetic energies of spallation nuclei and light particles and nuclei are more meager, but in one comparison in a biological situation Armstrong and Bishop⁸ find good agreement between calculated and measured radiation doses. Consequently, except possibly for the matter of helium production, the NMTC inputs to the present calculation might be estimated to be accurate to about a factor of two; and for "integrated" quantities such as the total damage energy or total spallation nucleus cross sections, the accuracy is likely to be significantly greater than this.

In the calculation being described here it was assumed that 800-MeV protons were incident normally on a natural-isotopic-mixture copper disc 1 cm thick and so large in radius (50 cm) as to preclude escape of charged particles from the target sides. The particular target thickness used was chosen because it was small enough to make particle production and energy deposition uniform (within statistical error) throughout the target, but large enough to ensure that a reasonable fraction (about 8%) of the incident protons actually had nuclear interactions within the target. The neutron cutoff energy was specified as 15 MeV, and the proton cutoff energy as 20 MeV; the charged pion cutoff energy is obtained automatically in the program from that of the proton by scaling according to mass. Calculations were made for seventeen statistically independent batches of 20 000 protons each, for a total of three hundred and forty thousand 800-MeV protons incident on the target. Statistical fluctuations in the average numbers and energies of neutrons, light nuclei, and significant spallation nuclei with the inclusion of results from new batches had become small (about 3%) after incorporation of data from all seventeen batches, though new low-probability spallation nuclei were still appearing in each new batch.

Data were collected from those NMTC events in which a particle emerged from the backside of the target, a charged particle dropped below cutoff energy in the target, or a nuclear interaction oc-

curred. In the latter case the type and kinetic energy of the spallation nucleus and of each light particle/nucleus produced in the cascade or evaporation were recorded. In addition, an energy histogram entry was made for each light particle/nucleus, and the energy squared of the spallation nucleus was tabulated. At the end of the batch run appropriate averages were taken, and the results of the individual batches were later incorporated into a single overall set of averages in a separate calculation. Data were retained only for spallation nuclei with $26 \leq A \leq 65$, and for a given A with Z values satisfying $-5 \leq Z - [A/2] \leq 4$, where $[A/2]$ is the greatest integer in $A/2$. Spallation nuclei were produced with every A value in the indicated range, and undoubtedly were produced with $A \leq 26$ also. However, the average numbers of spallation nuclei per incident proton for A values toward the bottom of the above range were quite small, and the NMTC results for cross sections and energies there are suspect in any case.

In Table I are shown the average numbers of particles escaping the back surface of the 1-cm-thick target per incident proton, and the average kinetic energy per incident proton carried away by each type of particle. It is seen that essentially one proton exits the back surface of the target for each proton incident on the front surface. Table II shows the average numbers and production cross sections for the spallation nuclei (without regard to type), neutrons, and light nuclei produced within the 1-cm-thick

TABLE I
AVERAGE NUMBERS AND ENERGIES OF PARTICLES
ESCAPING THE BACK SURFACE OF THE TARGET

Particle	Average Number Escaping Back Surface Per Incident Proton	Average Total Energy Carried Away Per Incident Proton (MeV)
p	0.999	751
n	0.112	15.0
π^+	0.0074	0.96
π^-	0.0020	0.20

TABLE II
AVERAGE NUMBERS AND ENERGIES OF NEUTRONS AND
NUCLEI PRODUCED IN THE TARGET

Particle/ Nucleus	Average Number Per Incident Proton	Production Cross Section (b)	Average Kinetic Energy Per Incident Proton (MeV)
All Spalla- tion Nuclei	0.087	1.03	0.20
p	0.22	2.53	2.45
n	0.29	3.42	1.38
² H	0.020	0.23	0.23
³ H	0.0038	0.04	0.05
³ He	0.0021	0.03	0.04
⁴ He	0.014	0.16	0.20

target, as well as the average kinetic energy per incident proton for each type particle/nucleus. The energy per proton not accounted for in Tables I and II has gone into electronic excitation in the material, pion production (mass energy for escaping charged pions, and mass and kinetic energy for neutral and charged pions decaying in the target), and nuclear binding energy supplied in the process of nuclear spallation. It is seen that there is copious proton and neutron production in the target, and significant helium production as well. (Recall that, according to previous discussion, the calculated helium production cross section is probably low by a factor two or more.)

More than one hundred, fifty different nuclides were generated in the computer-simulated bombardment, most of them unstable but those appearing in significant numbers generally having half-lives of seconds or longer. A three-dimensional-perspective plot of nuclide production cross sections as a function of A and Z is given in Fig. 1, and the nuclides and their production cross sections are listed in Table III in order of decreasing cross-section size. It is interesting to note that production cross sections fall off rather slowly as one moves down the list, the twenty largest cross sections summing to slightly less than two-thirds the total spallation nucleus production cross section.

The calculated average initial kinetic energies of the spallation nuclei range from a low of about

Fig. 1. Calculated production cross section for the spallation nuclei as a function of A and Z.

120 keV for ⁶⁵Ni to a high of more than 16 MeV for ³⁴P, and are shown graphically as functions of A and Z in Fig. 2. A more important quantity is the average kinetic energy of each nuclear species per incident proton, i.e., the product of the average kinetic energy of each nuclear species and the average number of nuclei of that type produced per incident proton. This quantity is shown graphically as a function of A and Z in Fig. 3, and in tabular form in order of decreasing average energy in Table IV. The fall-off is even slower as one moves down the list for the average nuclide kinetic energies per incident proton than for the production cross sections, the first twenty nuclides in Table IV accounting for only half the average kinetic energy of 200 keV deposited in spallation nuclei per incident proton. It is seen that the greatest amounts of kinetic energy are deposited in nuclear species

Fig. 2. Spallation nucleus average kinetic energy as a function of A and Z.

TABLE III
PRODUCTION CROSS SECTIONS FOR THE SPALLATION
NUCLEI, IN DECREASING ORDER

<u>Nuclide</u>	<u>Cross Section (mb)</u>	<u>Nuclide</u>	<u>Cross Section (mb)</u>	<u>Nuclide</u>	<u>Cross Section (mb)</u>	<u>Nuclide</u>	<u>Cross Section (mb)</u>
⁶² Cu	91	⁴⁹ V	15	³⁶ Cl	5.0	⁴⁹ Ti	2.1
⁶² Ni	64	⁵⁰ Cr	14	³⁷ A	4.8	³⁷ Cl	2.0
⁶⁰ Ni	47	⁶³ Ni	14	⁵⁵ Co	4.8	⁶² Zn	2.0
⁶¹ Ni	41	⁵⁴ Mn	13	⁴⁶ Sc	4.7	⁶³ Co	1.9
⁵⁹ Ni	36	⁵² Cr	11	⁵¹ Mn	4.6	⁵⁶ Mn	1.9
⁶¹ Cu	34	⁴⁴ Sc	11	³⁵ Cl	4.3	⁴⁷ Sc	1.8
⁶⁴ Cu	34	⁴⁵ Sc	10	⁶³ Zn	4.3	³⁸ K	1.7
⁶³ Cu	33	⁵⁰ V	9.3	⁴⁷ V	4.2	⁴² K	1.7
⁵⁵ Fe	30	⁴² Ca	8.9	⁴³ Sc	4.1	⁴⁰ Ca	1.7
⁵⁷ Co	29	⁴³ Ca	8.5	⁴¹ K	4.0	⁶⁵ Zn	1.7
⁵³ Mn	25	⁶⁰ Co	8.4	⁵⁵ Mn	3.7	⁴⁵ Ca	1.6
⁵⁸ Co	24	⁵⁷ Fe	8.0	⁵⁸ Fe	3.4	³⁹ A	1.3
⁶⁴ Ni	23	⁴¹ Ca	7.5	⁴⁴ Ca	3.2	⁴⁴ Ti	1.2
⁵⁶ Co	22	³⁹ K	7.5	⁵³ Fe	3.2	²⁹ Si	1.2
⁵¹ Cr	21	⁴⁹ Cr	7.3	³⁴ S	3.2	³⁴ Cl	1.2
⁵⁴ Fe	21	⁶⁰ Cu	7.0	³³ S	3.0	⁴⁶ V	1.1
⁵² Mn	20	⁶⁵ Cu	6.9	⁵³ Cr	3.0	⁵⁹ Fe	1.1
⁵⁸ Ni	20	⁴⁰ K	6.6	⁵¹ V	2.8	⁵⁹ Cu	1.1
⁴⁸ V	18	⁴⁸ Ti	6.3	⁶² Co	2.7	⁶⁰ Fe	1.1
⁴⁶ Ti	17	⁶¹ Co	6.0	³¹ P	2.5	³⁰ P	1.0
⁴⁷ Ti	15	⁴⁵ Ti	5.9	⁶⁵ Ni	2.3	⁴² Sc	1.0
⁵⁶ Fe	15	³⁸ A	5.8	³² P	2.3		
⁵⁹ Co	15	⁵⁷ Ni	5.2	⁶⁴ Zn	2.2		

having A and Z values several units below those of copper. However, in the next section we shall find that because of charge and mass mismatches with target atoms, the nuclear species receiving the most average kinetic energy per incident proton from reactions are not the ones which produce the most lattice damage.

Energy distribution histograms for the nucleons and light nuclei produced in the copper target, determined from the energies these particles possess when

NMTC stops transporting them, are shown in Fig. 4 (a-f). The sharp cutoffs in the proton and neutron spectra at 20 and 15 MeV, respectively, are artifacts of the structure of the computer program, which transports the nucleons--allowing them to have nuclear interactions--until their energies drop to these values, where they are "picked up" by the analysis code for later investigation of radiation damage effects. The spike in the proton distribution in the 19-20 MeV bin arises from those protons which

TABLE IV
AVERAGE KINETIC ENERGIES PER PROTON FOR THE
SPALLATION NUCLEI, IN DECREASING ORDER

Nuclide	Average Energy Per Proton (keV)	Nuclide	Average Energy Per Proton (keV)	Nuclide	Average Energy Per Proton (keV)	Nuclide	Average Energy Per Proton (keV)	Nuclide	Average Energy Per Proton (keV)
⁴⁶ Ti	7.3	⁵⁴ Mn	2.9	⁶³ Cu	0.91	⁶³ Ni	0.34	³² Si	0.08
⁴⁸ V	6.9	⁵⁸ Co	2.8	⁴² K	0.90	⁵⁸ Fe	0.33	⁶⁴ Zn	0.08
⁵¹ Cr	6.1	³⁴ S	2.7	³⁰ P	0.88	³⁰ Si	0.32	⁴² Ti	0.08
⁵³ Mn	6.0	⁴⁹ Cr	2.6	⁵³ Cr	0.86	²⁸ Al	0.32	⁴⁴ K	0.07
⁴⁷ Ti	5.8	³³ S	2.6	⁵⁵ Co	0.82	⁴³ K	0.31	⁵⁵ Cr	0.07
⁵⁵ Fe	5.4	⁵⁶ Fe	2.4	⁴⁹ Ti	0.80	⁵⁶ Mn	0.27	⁵⁶ Ni	0.07
⁴⁹ V	5.4	⁴⁸ Ti	2.3	⁵¹ Fe	0.77	⁶⁴ Ni	0.26	³⁰ Al	0.07
⁴² Ca	5.2	⁴¹ K	2.3	³⁹ Ar	0.76	⁴¹ Ar	0.23	⁴⁹ Sc	0.06
⁴⁴ Sc	5.2	⁵⁸ Ni	2.3	⁵⁷ Ni	0.76	⁶¹ Co	0.23	⁵⁸ Mn	0.06
³⁹ K	5.0	⁴³ Sc	2.3	³² S	0.73	²⁶ Al	0.21	²⁸ S	0.06
⁴³ Ca	4.9	³¹ P	2.3	⁴⁵ Ca	0.68	⁵⁰ Mn	0.19	⁵⁴ Co	0.06
⁵² Cr	4.9	⁶² Cu	2.2	⁴⁷ Sc	0.68	⁵⁰ Ti	0.18	⁶⁰ Fe	0.05
⁵⁰ Cr	4.6	⁴⁶ Sc	2.1	⁴⁴ Ti	0.61	³⁹ Ca	0.18	²⁶ P	0.05
⁵⁴ Fe	4.4	³² P	2.0	³³ P	0.59	⁴⁶ Ca	0.17	⁵³ V	0.05
⁴⁵ Sc	4.3	⁶¹ Ni	1.8	⁶⁴ Cu	0.58	⁴⁸ Sc	0.14	⁴⁵ V	0.04
⁴¹ Ca	4.2	⁴⁷ V	1.7	³⁵ S	0.58	⁵⁴ Cr	0.13	⁶³ Co	0.04
⁵⁷ Co	4.1	³⁷ Cl	1.6	⁵⁵ Mn	0.57	⁶³ Zn	0.12	⁴³ Ti	0.04
⁵⁶ Co	3.7	⁶¹ Cu	1.6	⁶⁰ Co	0.56	³⁶ S	0.12	⁴⁹ Mn	0.04
⁴⁰ K	3.7	⁴⁴ Ca	1.5	⁴⁰ Ar	0.54	⁵² Fe	0.12	⁴⁶ Cr	0.03
³⁸ Ar	3.5	⁵¹ Mn	1.5	⁴² Sc	0.51	⁶² Co	0.11	⁴⁰ Cl	0.03
³⁶ Cl	3.3	⁶² Ni	1.3	²⁷ Al	0.51	⁵² V	0.11	³⁵ Ar	0.03
⁵⁹ Ni	3.3	⁵⁹ Co	1.2	²⁸ Si	0.50	⁵⁹ Fe	0.11	⁴⁷ Ca	0.03
⁴⁵ Ti	3.2	³⁴ Cl	1.2	⁶⁰ Cu	0.47	²⁶ Mg	0.10	⁶⁵ Zn	0.03
³⁵ Cl	3.2	²⁹ Si	1.2	⁴⁶ V	0.46	⁶⁵ Cu	0.10	⁴⁷ Cr	0.03
³⁷ Ar	3.1	³⁸ K	1.1	³⁶ Ar	0.46	⁵⁷ Mn	0.09	⁴² Ar	0.03
⁵² Cr	3.1	⁵⁷ Fe	1.1	⁴⁸ Cr	0.42	³¹ Si	0.09	⁴² V	0.03
⁶⁰ Ni	2.9	⁴⁰ Ca	1.0	³⁸ Cl	0.38	⁶² Zn	0.09	³⁸ Ca	0.03
⁵⁰ V	2.9	⁵¹ V	0.94	³⁴ P	0.34	⁵⁹ Cu	0.08	⁵³ Co	0.03

Fig. 3. Spallation nucleus kinetic energy cross section as a function of A and Z.

are dropped by NMTC when their energies fall below the 20-MeV cutoff because of electronic stopping effects. For the remaining four light nuclei the energy distributions were tabulated for forty 1-MeV-wide bins, and all nuclei with kinetic energies above 40 MeV were placed in the 39-40-MeV bin. From the "bumps" in this bin for ^3H , ^3He , and ^4He , it is seen that a small percentage of these nuclei were produced with energies above 40 MeV.

Calculated average kinetic energies for the neutron and for the light nuclei are given in Table V. It should be noted that the averages for protons and neutrons are based only on those particles which have energies below 20 and 15 MeV, respectively.

TABLE V

CALCULATED AVERAGE KINETIC ENERGIES FOR THE NEUTRON AND LIGHT NUCLEI. FIGURES FOR THE PROTON AND NEUTRON INCLUDE ONLY PARTICLES WITH ENERGIES BELOW 20 AND 15 MeV, RESPECTIVELY

Nucleon/Nucleus	Average Kinetic Energy (MeV)
p	11
n	4.8
^2H	11
^3H	12
^3He	17
^4He	15

III. DAMAGE ENERGY DETERMINATION

It is necessary to determine the damage effects produced by the spallation nuclei, light nuclei, and neutrons generated in the nuclear interactions initiated by the 800-MeV protons. For this purpose it will be assumed that the target is thick enough so that essentially all spallation nuclei and below-cutoff-energy light nuclei produced in the interior of the target stop within the target, an assumption certainly well justified in the case of the 1-cm-thick copper target for which the calculation was performed. The damage energy for each such nucleus with the calculated energy spectrum determined by NMTC can then be computed and multiplied by the average number of nuclei of this type produced per incident proton, and these average damage energies per incident proton summed over nuclear type to obtain the average total damage energy produced in the 1-cm-thick copper target per incident proton by all the spallation and light nuclei generated in the target. Because of the 1-cm target thickness, this damage energy per incident proton can be divided by the number of copper atoms per unit volume to obtain a partial damage energy cross section. This partial damage energy cross section can then be utilized to determine that part of the damage energy due to energetic nuclei which will be produced by 800-MeV protons in copper targets of other thicknesses, provided these thicknesses satisfy the conditions of being

1. small enough so that damage as a function of depth is essentially uniform;
2. large enough so that essentially all spallation and below-cutoff light nuclei produced stop in the target.

Actually, it will be seen below that the light nuclei produce so little damage compared to the spallation nuclei that they can be ignored for damage energy purposes. Condition 2 can then be weakened to require only that essentially all spallation nuclei stop in the target, a requirement well satisfied for target thicknesses equal to or greater than 10^{-2} cm. This form of condition 2 will therefore hold in most cases of interest.

Suppose, then, that one has a projectile atom with charge and mass numbers Z_1 , A_1 , and initial energy E_0 moving in a monatomic material characterized by Z_2 , A_2 . One wishes to determine the part $\hat{E}(E_0)$ of

Fig. 4. Energy histograms for the neutron and light nuclei: (a) proton; (b) neutron; (c) deuterium; (d) tritium; (e) ^3He ; (f) ^4He .

the energy E_0 which will be transformed into kinetic energy of the nuclei in the target material as the projectile atom is stopped. This energy, the so-called damage energy, can produce atomic displacements and therefore lattice damage, while the remaining energy $E_0 - \hat{E}(E_0)$ goes into electronic excitation which is unlikely to produce damage effects. The approximation will be made that energy losses of the projectile atom to lattice nuclei and to lattice electrons are uncorrelated. Let $\frac{d\sigma}{dT}(T, E)$ be the differential cross section for a projectile atom of energy E to transfer a (laboratory) kinetic energy T to a target nucleus, $T_M(E)$ the maximum T possible for a given E , N the number density of target atoms, and $L(T)$ the fraction of the energy T that a target nucleus of energy T will itself distribute to other target nuclei as it is brought to a stop in the target material. Then the damage energy resulting from the projectile atom of energy E moving a distance dx through the target is

$$N dx \int_0^{T_M(E)} L(T) \frac{d\sigma}{dT}(T, E) dT. \quad (1)$$

As the projectile atom moves through the target material its energy decreases, so that E in expression (1) can be regarded as a function of x . The total damage energy produced as the projectile atom stops is obtained by summing expressions of the form (1) along its entire trajectory:

$$\hat{E}(E_0) = N \int_0^{x_0} dx \int_0^{T_M(E(x))} L(T) \frac{d\sigma}{dT}(T, E(x)) dT \quad (2)$$

$$= N \int_0^{E_0} dE \frac{1}{\left| \frac{dE}{dx} \right|} \int_0^{T_M(E)} L(T) \frac{d\sigma}{dT}(T, E) dT, \quad (3)$$

where in (2) x_0 is the range of the projectile atom.¹¹ Expression (2) (or (3)) assumes a fixed range, and so does not treat properly those collisions in which the energy T transferred to a struck atom is comparable in size to E ; but the cross section for such events is small, and the error produced by using this expression is rather insignificant (probably an overestimate of $\hat{E}$ by not more than 2% in the present calculation--see the discussion of

$\hat{E}(E)/E$ for ^{65}Cu below). The stopping power $\left| \frac{dE}{dx} \right|$ appearing in the form (3) of the expression is the sum of the electronic and nuclear stopping powers,

$$\left| \frac{dE}{dx} \right| = S_n(E) + S_e(E), \quad (4)$$

where

$$S_n(E) = N \int_0^{T_M(E)} T \frac{d\sigma}{dT}(T, E) dT. \quad (5)$$

Determination of an appropriate form for $\frac{d\sigma}{dT}(T, E)$ is a complicated matter, as is the calculation of a suitable $S_e(E)$. Once these functions are known for appropriate choices of Z_1 , A_1 , Z_2 , and A_2 , $S_n(E)$ and $L(T)$ can be calculated in a straightforward fashion, and $\hat{E}(E_0)$ calculated from Eq. (2) or (3).

Forms for $\frac{d\sigma}{dT}$ and S_e , and the resulting S_n and L , have been given by Lindhard and various coauthors in Refs. 3-5 for a Thomas-Fermi model. The authors introduce³ a scaled projectile energy ϵ and energy transfer $t^{1/2}$ in the forms

$$\epsilon = \frac{a}{Z_1 Z_2 e^2} \cdot \frac{1}{2} M_0 v^2, \quad (6)$$

$$t = TE \frac{M_2}{M_1} \left[\frac{a}{2Z_1 Z_2 e^2} \right]^2 = \epsilon^2 \sin^2 \frac{\theta}{2}, \quad (7)$$

where M_0 is the reduced mass of the two-atom system, v their relative speed, θ the center-of-mass scattering angle, and a a screening length given approximately by

$$a = \frac{0.8853 a_0}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}} \quad (8)$$

with a_0 the Bohr radius. In terms of these quantities they write an approximate "universal" scattering cross section

$$\frac{d\sigma}{dT} = \frac{\pi a^2}{2t} f(t^{1/2}), \quad (9)$$

where $f(t^{1/2}) \approx (2t^{1/2})^{-1}$ for $t^{1/2} \geq 40$, $f(t^{1/2}) \approx 1.43(t^{1/2})^{0.35}$ for $t^{1/2} \leq 0.002$, and $f(t^{1/2})$ is given by the authors in tabular form for $0.002 \leq t^{1/2} \leq 40$.

The authors then introduce a reduced range ρ in terms of the range R along the path and other quantities as

$$\rho = \pi N \cdot 4\pi z^2 \frac{M_1 M_2}{(M_1 + M_2)^2}, \quad (10)$$

and a "universal" scaled specific nuclear stopping power $s(\epsilon)$,

$$s(\epsilon) = \frac{1}{\epsilon} \int_0^\epsilon f(\zeta) d\zeta, \quad (11)$$

such that the total nuclear stopping power of Eq. (5) is

$$S_n(E) = \frac{E}{\epsilon} \frac{\rho}{R} s(\epsilon). \quad (12)$$

In Ref. 4 the authors report on results of consideration of electronic stopping in a Thomas-Fermi picture. They conclude that as long as the speed v of the projectile atom is less than $v_1 = v_o Z_1^{2/3} \equiv \frac{e^2}{h} Z_1^{2/3}$ the electronic stopping power is proportional to v , and in fact

$$S_e = N \cdot \xi_e \cdot 8\pi e^2 a_o \frac{Z_1 Z_2}{Z} \frac{v}{v_o}, \quad (13)$$

where

$$Z = (Z_1^{2/3} + Z_2^{2/3})^{3/2} \quad (14)$$

and ξ_e is a constant of order $Z_1^{1/6}$. The authors remark that a precise proportionality to v will not hold over the entire velocity range $v < v_1$, but that at some point the stopping power will begin to increase more slowly with v and for large enough v ($> v_1$) will be a decreasing function of v . The kinetic energy corresponding to v_1 is about 25 keV for a proton, 250 keV for ^4He , 21 MeV for ^{27}Al , and 140 MeV for ^{65}Cu . For the spallation nuclei, therefore, it may be assumed that S_e is velocity proportional along the entire stopping trajectory, and expression (13)

with $\xi_e \approx Z_1^{1/6}$ was used in the calculation described here. Treatment of the light nuclei will be discussed later.

For the case $A_1 = A_2$, $Z_1 = Z_2$ one has $\hat{E}(E_o) = E_o L(E_o)$ by the definition of L , and Eq. (3) reduces to an integral equation

$$E_o L(E_o) = N \int_0^{E_o} \frac{1}{|dE/dx|} dE \int_0^{E_o - TL(T)} \frac{d\sigma}{dT}(T, E) dT \quad (15)$$

from which $L(T)$ can be determined. In Ref. 5 Lindhard et al. determine L for the cross section (9) and electronic stopping (13) from an integral equation similar to (15) but incorporating modifications intended to treat the case where T is comparable to E more accurately. They represent their results in the form

$$L(\epsilon) = \frac{1}{1 + k \cdot g(\epsilon)}, \quad (16)$$

where

$$k = 0.133745 \frac{Z^{2/3}}{A^{1/2}}, \quad (17)$$

and $g(\epsilon)$ is given graphically. Subsequently Robinson¹² gave an analytic approximation

$$g(\epsilon) = 3.400\epsilon^{1/6} + 0.40244\epsilon^{3/4} + \epsilon \quad (18)$$

to the numerically-determined function of Lindhard et al. In the current application k was calculated with an average A for the two copper isotopes.

Equations (2) (or (3)), (4), (9), (12), (13), (16), and (18) may be combined to calculate the damage energy functions $\hat{E}(E)$ in copper for the various spallation nuclei generated by NMTC. This was done here by using Eq. (2) for the damage energy. First a position-versus-energy function was calculated for a spallation nucleus with an initial energy of 30 MeV, using a Runge-Kutta routine down to the region of ϵ small enough so that small- ϵ analytic expressions for f and s in (9) and (12) were available and the integration could be completed analytically. The double integration was then performed for a number of E_o values from 0 to 30 MeV by using three- and four-point

polynomial interpolation and integration procedures. Damage efficiencies $\hat{E}(E_0)/E_0$ were also determined for the various spallation nuclei from these results.

In actual fact not all kinetic energy transferred to lattice nuclei is effective in producing damage; since a certain average minimum energy E_{disp} is required to displace a lattice atom from its site, an energy $T < E_{\text{disp}}$ transmitted to a nucleus will in general be dissipated as heat energy and not contribute to lattice damage. An attempt to partially estimate this effect was made by taking the T and range integrations in (2) not to zero but to a (rather modest) cutoff energy of 10 eV.¹³ The estimate of the effect is partial because no such cutoff is contained in $L(T)$ itself. The result of introducing the cutoff may be determined from Table VI, which shows both the calculated damage efficiency for ^{65}Cu and the Lindhard function $L(E)$ for copper for several values of the energy. It is known that the function $L(E)$ satisfying (15) lies slightly above that given by (16), (18), so the damage efficiency calculated for copper from (2) with no cutoff involves a "mixture" of the two functions and should lie slightly above the $L(E)$ from (16), (18). From Table VI one sees that the calculated damage efficiency with the cutoff at 10 eV does indeed lie slightly above $L(E)$ for energies above a few tens of keV. However, it falls below $L(E)$ for lower energy values, reaching

TABLE VI

COMPARISON OF THE CALCULATED $\hat{E}(E)/E$
(WITH CUTOFF) FOR ^{65}Cu AND THE LINDHARD
FUNCTION $L(E)$ FOR COPPER

Energy (MeV)	$L(E)$	$\hat{E}(E)/E$
0.001	0.820	0.718
0.002	0.801	0.739
0.005	0.774	0.744
0.01	0.750	0.735
0.05	0.678	0.680
0.1	0.635	0.640
1	0.386	0.382
10	0.0984	0.0999

Fig. 5. Damage energy of ^{65}Cu in natural copper.

a maximum at about 5 keV and then of course decreasing toward zero for $E \rightarrow 0$ while $L(E) \rightarrow 1$. Over the energy ranges of interest in the present calculation, however, the damage efficiency calculated with the cutoff is essentially the same as $L(E)$, so that introduction of the cutoff has negligible effect on the calculated damage energies.

A plot of the damage energy $\hat{E}(E)$ for ^{65}Cu is shown in Fig. 5. The damage energy curves for all of the spallation nuclei are qualitatively similar to this one. It should be noted that in the 1 to 10 MeV range where the average kinetic energies of most of the spallation nuclei lie, a factor two increase in energy produces a fractional decrease of about one-third in the damage energy; and this approximate ratio holds for the other spallation nuclei as well. Thus the average damage energy per proton for a given nuclide depends somewhat more strongly on the nuclide's production cross section than on its average kinetic energy.

Variation of the damage efficiency $\hat{E}(E)/E$ with Z for fixed A is not large, as may be seen by comparing Figs. 6(a) and (b) which show the damage efficiency curves for $A = 65$, $Z = 31$ (^{65}Ga) and a hypothetical nucleus $A = 65$, $Z = 27$ (^{65}Co), respectively. (The Z values actually occurring in the calculation for $A = 65$ are 28, 29, 30.) The damage efficiency for the lower charge nucleus is larger at 5 keV by less than 1%, the two curves cross between 200 and

Fig. 6. Damage efficiency in natural copper for (a) ^{65}Ga and (b) ^{65}Co .

300 keV, and the damage efficiency for the higher charge nucleus is larger at 10 MeV by about 7%. To show the variation in damage efficiency over the range of A values covered by the calculation, Fig. 7(a) gives the damage efficiency curve for $A = 65$, $Z = 29$ (^{65}Cu), and Fig. 7(b) that for $A = 26$, $Z = 13$ (^{26}Al). The damage efficiency for the $A = 65$ atom is 13% higher at 5 keV, 42% higher at 100 keV, 180% higher at 1 MeV, and more than 300% higher at 10 MeV. The physical reason for this behavior is, of course, that the strengths of nuclear and electron Coulomb interactions for a projectile atom vary in fairly

Fig. 7. Damage efficiency in natural copper for (a) ^{65}Cu and (b) ^{26}Al .

similar ways as Z is varied with A fixed, but the average fraction of kinetic energy transferred in a single nuclear Coulomb scattering decreases (because of mass mismatch) as A decreases with Z fixed, while the average kinetic energy transferred in an electron collision increases. Combining these two behaviors yields increased transfer of energy to electrons relative to nuclei also in the case where A and Z decrease in fixed ratio.

As mentioned in the last section, the average energy and average squared energy for each nuclide produced were computed from the NMTC results. The

TABLE VII

PARTIAL DAMAGE ENERGY CROSS SECTIONS FOR THE
SPALLATION NUCLEI, IN DECREASING ORDER

Nuclide	Damage energy cross section (barn-keV)	Nuclide	Damage energy cross section (barn-keV)	Nuclide	Damage energy cross section (barn-keV)	Nuclide	Damage energy cross section (barn-keV)
⁶² Cu	14.5	⁵⁶ Fe	6.2	⁵¹ Mn	2.1	⁴⁹ Ti	0.9
⁶⁰ Ni	12.9	⁵³ Cu	5.7	⁵⁷ Ni	2.1	³⁴ S	0.9
⁵⁵ Fe	12.6	⁵⁴ Mn	5.7	⁶⁴ Ni	2.1	³³ S	0.8
⁵⁹ Ni	12.1	⁵² Cr	5.0	⁶⁰ Cu	2.0	⁶³ Zn	0.8
⁵⁷ Co	11.5	⁵⁹ Co	4.7	⁵⁵ Co	2.0	⁶⁵ Cu	0.8
⁵³ Mn	11.1	⁴⁴ Sc	4.2	⁴⁶ Sc	1.9	⁵⁶ Mn	0.8
⁵¹ Cr	9.3	⁶⁴ Cu	4.2	³⁸ A	1.9	⁴⁷ Sc	0.7
⁶¹ Ni	9.2	⁵⁰ V	4.1	⁴⁷ V	1.8	⁴⁵ Ca	0.7
⁵⁶ Co	9.2	⁴⁵ Sc	4.0	⁴³ Sc	1.7	³¹ P	0.7
⁵⁴ Fe	9.1	⁴² Ca	3.4	⁴¹ K	1.7	⁴⁰ Ca	0.7
⁵⁸ Co	9.0	⁴³ Ca	3.4	³⁷ A	1.5	³⁷ Cl	0.7
⁶² Ni	8.9	⁴⁹ Cr	3.3	³⁶ Cl	1.5	⁴² K	0.6
⁵² Mn	8.6	⁵⁷ Fe	3.0	⁵⁵ Mn	1.4	³⁸ K	0.6
⁶¹ Cu	8.1	⁴¹ Ca	2.8	⁵³ Fe	1.4	⁶² Co	0.6
⁴⁸ V	7.8	³⁹ K	2.8	⁵³ Cr	1.4	³² P	0.6
⁵⁸ Ni	7.4	⁴⁸ Ti	2.8	⁶¹ Co	1.3	⁴⁶ V	0.5
⁴⁶ Ti	7.1	⁴⁵ Ti	2.6	⁵¹ V	1.3	⁴⁴ Ti	0.5
⁴⁹ V	6.5	⁶⁰ Co	2.4	³⁵ Cl	1.3	⁶² Zn	0.5
⁴⁷ Ti	6.4	⁴⁰ K	2.3	⁴⁴ Ca	1.3	³⁹ A	0.5
⁵⁰ Cr	6.4	⁶³ Ni	2.2	⁵⁸ Fe	1.1		

rms energy spread ΔE was calculated from these quantities, and the energy spectrum was assumed to be a Gaussian with the same average energy and ΔE . The average damage energy per nuclide was then calculated from this energy spectrum and the calculated damage energy function for the nuclide, using a five-point Gauss-Hermite quadrature. From this quantity and the average number of nucleons of the species produced per incident proton an average damage energy per proton for the nuclide was calculated, and division by the number density of copper atoms yielded a partial damage energy cross section for the nuclide. The

partial damage energy cross sections for the various nuclear species are given in Table VII in order of decreasing cross section. The total damage energy cross section for all spallation nuclei is 320 barn-keV, and the first twenty nuclides shown in Table VII contribute just under 60% of this total. On comparing Tables IV and VII one notes a considerable re-ordering, with lighter nuclei in Table IV falling to lower positions in Table VII to be replaced by heavier nuclei with lower average kinetic energies per proton but greater damage efficiencies. It is interesting to note that the two nuclei with greatest

damage energy cross sections in Table VII are not even among the first twenty entries in Table IV (being 40th and 27th, respectively, in average kinetic energy per incident proton).

Determination of the damage energies for the light nuclei was somewhat complicated by the fact that the range of validity of expression (13) for the electronic stopping power covers only a very small part of the energy region of interest. In a somewhat higher energy range, whose upper limit is well above the energy intervals of interest here, the electronic stopping power is given by the Bethe formula

$$S_e = \frac{4\pi e^4}{m_e c^2} N Z_1 Z_2^2 \left[\frac{1}{\beta^2} \ln \frac{2m_e c^2 \beta^2}{I(1-\beta^2)} - 1 \right], \quad (19)$$

where m_e is the electron mass, c the speed of light, β is v/c , and I is an appropriate ionization potential for the target atoms. For the present calculation a value $I = 320$ eV was used, based on the results of a study by Janni.¹⁴ As β decreases toward zero from sufficiently small values the right-hand side of (19) first increases with positive second derivative, passes through an inflection point and then a maximum, and finally decreases and becomes negative for some $\beta > 0$. The expression ceases to accurately represent the electronic stopping power in the β range between the maximum and the inflection point. The interval between the upper limit of validity of Eq. (13) and the lower limit of validity of Eq. (19) is one where the physical phenomena responsible for electronic energy loss are very complex, and no satisfactory "first principles" theoretical expression for S_e in this range exists. In order to have a convenient analytic expression for S_e in this interval an interpolation was made between the upper limit of the range where (13) was employed and the lower limit of the range where (19) was employed with a cubic polynomial, the coefficients of the polynomial being determined by the requirement that S_e and its first (velocity) derivative be continuous at each end of this interval. The precise values of S_e in the interval could be varied somewhat by adjusting the particular choice of end points for the interval, and it was found that if the upper limit for use of (13) was chosen as $0.8 v_1$ and the lower limit for use of (19) as 0.89

times the value of β at the inflection point then the interpolating polynomial agreed with experimental data within its interval of use to 3% or better for the proton, and to greater accuracy for ^4He . It was also found that calculated damage energy functions for these two nuclei were quite insensitive in regions of interest to considerable variations in the choice of the two cutoff points, so the same cutoffs were used for ^2H and ^3H . Because of the unusual charge-mass ratio for ^3He , this choice of cutoffs produced a damage energy curve with a local maximum and minimum in the intermediate region, so the cutoffs for this nucleus were taken as $0.7 v_1$ below and 0.707 times the inflection-point β above. This change in the case of ^3He was made for purely esthetic reasons, the effect on the calculated damage energy function in the region of interest being insignificant.

Because of the large mass mismatch, the damage efficiency for ^4He is low, as seen in Fig. 8(a). The mismatch is most extreme for the proton, whose damage efficiency curve is given in Fig. 8(b). Curves for ^2H , ^3H , and ^3He are intermediate between the two shown. Average damage energies per incident proton were obtained for each of the light nuclei by calculating the integral of the product of the damage energy function and the appropriate energy distribution shown in Fig. 4 and multiplying by the number of nuclei of this type produced per incident proton. The result was then converted to a partial damage energy cross section by dividing by the number density of target atoms, and these damage energy cross sections are shown in Table VIII. It is seen that though the light nuclei receive about fifteen times as much kinetic energy per incident proton as the heavier spallation nuclei, the damage energy they produce is more than forty times less because of their extremely low damage efficiencies.

All the foregoing damage energy calculations depend for their accuracy on the accuracy of the so-called LSS theory of Lindhard *et al.* The LSS stopping power and collision cross section seem to yield ranges and damage distributions varying from good agreement with experiment to differences by less than a factor 2.^{12,15,16} The LSS stopping power may be less accurate for the light nuclei, but is used over only a small part of their energy range. Overall, then, the damage energies calculated here are probably correct to within a factor less than 2.

Fig. 8. Damage efficiency in natural copper for (a) ^4He and (b) ^1H .

Furthermore, one of the most important uses of the damage energy cross sections calculated here will be in comparisons with damage energy cross sections for neutrons and other bombarding particles, and these other damage energy cross sections are usually also calculated by use of the LSS theory. In such comparisons errors in the Lindhard theory will tend to cancel, so that the ratio of damage energies from two different sources will tend to be more accurate than the damage energies themselves. There is some experimental evidence that the LSS damage energy is capable of correlating damage effects due to thermal neutrons with those due to fission neutrons, and

damage effects due to fission neutrons with those due to 10-20 MeV neutrons, to within a factor ~ 2 .¹⁷⁻¹⁹

Thus far no account has been given of the damage energy due to the neutrons produced in the target. In the 1 to 15 MeV range in which most of the neutron energies fall (Fig. 4(b)) the mean free path in copper is slightly more than 3 cm, so that for typical target sizes most neutrons will have zero or one collision before leaving the target volume of interest. The damage energy due to these neutrons can be calculated; but in contrast to the case of the damage energy from the light and spallation nuclei, no damage energy cross section independent of target geometry can be determined. One can, however, obtain a target-dependent damage energy and estimate its size in typical cases.

To begin it is necessary to determine the damage energy cross section for a single neutron with the energy spectrum of Fig. 4(b) having one collision with a copper nucleus. This cross section, which will be denoted by $\langle E_D \rangle$, was determined by use of the code DON developed by Parkin and Goland.⁶ DON uses cross sections from ENDF/B III or IV (elastic, inelastic, and $(n,2n)$, (n,p) , (n,t) , $(n,^3\text{He})$, (n,α) , when separately available) to calculate the nuclear recoil spectrum produced by a given neutron spectrum, and employs the Lindhard function $L(T)$ to determine the corresponding damage energy cross section. For the neutron energy spectrum of interest here the

TABLE VIII

PARTIAL DAMAGE ENERGY CROSS SECTIONS FOR THE FIVE LIGHT NUCLEI

<u>Nucleus</u>	<u>Damage energy cross section (barn-keV)</u>
p	4.73
^2H	0.83
^3H	0.24
^3He	0.20
^4He	1.70
-	--
Total	7.70

damage energy cross section in copper was found to be 140 barn-keV.

Now assume that the cross-sectional area of the incident proton beam which impinges on the target is A ; and let x, y be coordinates in the plane perpendicular to the beam direction and z the coordinate in the beam direction. For complete generality suppose that the beam is not necessarily uniform over the area A , and let $\rho(x,y)$ be the function giving the relative intensity and normalized so that

$$\int_A \rho(x,y) dx dy = A \quad (20)$$

ρ is then dimensionless, and $\rho=1$ for a uniform beam.

For the following discussion refer to Fig. 9, which assumes the proton beam is normally incident on a flat target which intercepts the full beam. Similar figures and arguments analogous to that below can be given for other cases. For the "thin" target situation being studied here the target volume in which radiation damage due to spallation nuclei will occur is to a very good approximation (fringing effects are small) just the part directly in the beam path; this part is bounded by the front and back target surfaces and the dashed lines in Fig. 9. Only the material in this volume will be of interest for

Fig. 9. Drawing of the experimental arrangement envisioned in the derivation of the "qualified" neutron damage energy cross section. The x - and y -axes are perpendicular to the beam direction, and the z -axis is in the beam direction.

radiation damage studies, so only damage energy deposited in this volume by the neutrons produced will be viewed here as of interest.

Because of the thinness of the target, each point in the target volume of importance will act as a "source" of neutrons with a source strength which is independent of z but varies with x, y as $\rho(x,y)$ does. More precisely, if σ_n is the total cross section for neutron production by an incident proton and ϕ_p the total number of protons/sec incident on the target then a volume dV at position x, y, z in the target will emit

$$\sigma_n \phi_p \frac{\rho(x,y)}{A} N dV \quad (21)$$

neutrons per second. (In general the neutrons will be emitted with some distribution in energy and angle that will be independent of position in the (thin) target. For present purposes it is sufficiently accurate to assume that the angular distribution is isotropic. Also, the neutron mean free path varies so little over the important part of the energy spectrum that it is enough to consider an "average" neutron. When this is not so, one must use appropriate differential cross sections in (21).) If linear dimensions for the significant target volume are not too large compared to the neutron mean free path of 3+ cm--say not larger than 1 to 2 cm--then one can ignore cases where neutrons have more than one collision in the volume. If $d(x,y,z)$ is the average distance from point (x,y,z) to the volume surfaces, taking into account the appropriate angular distribution for neutron emission, then the average damage energy deposited in the volume by a neutron originating at this point is

$$\langle E_D \rangle N d(x,y,z) \quad (22)$$

The total damage energy per second deposited in the volume is, from (21) and (22),

damage energy/sec

$$= \frac{\sigma_n \phi_p \langle E_D \rangle N^2}{A} \int_V \rho(x,y) d(x,y,z) dV \quad (23)$$

If this result is normalized to average proton flux Φ_p/A and number of target atoms NV in the volume of interest, one gets an approximate "neutron-produced damage energy cross section"

$$N\sigma_n \langle E_D \rangle = \left[\frac{1}{V} \int_V \rho(x,y,z) d(x,y,z) dV \right] . \quad (24)$$

The quantity in brackets in expression (24) is a volume-averaged effective distance $\bar{d}$ a neutron must travel to escape the volume,

$$\bar{d} = \frac{1}{V} \int_V \rho(x,y,z) d(x,y,z) dV . \quad (25)$$

For the current case $N\sigma_n \langle E_D \rangle = 40$ barn-keV/cm, so one obtains a geometry-dependent result

$$\begin{aligned} &\text{neutron-produced damage energy cross section} \\ &= (40 \text{ barn-keV/cm}) \times \bar{d}, \end{aligned} \quad (26)$$

where $\bar{d}$ is given by (25) and has units cm. For a target volume of interest all of whose linear dimensions are of order 1 cm $\bar{d}$ will be of order 0.5 cm. It is interesting to observe that one may alter the ratio of neutron-produced damage to spallation- and light nucleus-produced damage from essentially zero to about 10% by varying the size of the target.

When $\rho(x,y)$ is not constant the damage produced by the spallation and light nuclei will not be uniform over the target volume of interest. Even when $\rho(x,y) \equiv 1$, however, the neutron-produced damage will in general not be uniform. The damage energy deposited in the vicinity of the point (x,y,z) will be proportional to

$$J(x,y,z) = \int_V \frac{\rho(x',y',z')}{|\vec{r} - \vec{r}'|^2} dV' , \quad (27)$$

where $\vec{r}$ and $\vec{r}'$ are vectors with components (x,y,z) and (x',y',z') , respectively, and the integration is of course over the target volume in the beam. If the neutron angular distribution is anisotropic an appropriate angular distribution function at (x',y',z') must be inserted in the integral in (27). If the target is uniformly irradiated by the beam, and if furthermore the neutron angular distribution is

isotropic, then $J(x,y,z)$ in (27) differs from $d(x,y,z)$ only by a factor 4π .

A procedure parallel to that described above may be used to calculate geometry-dependent cross sections for other neutron properties. One need only replace $\langle E_D \rangle$ in (24) by the appropriate alternate spectrum-averaged cross section. This fact will be used in Table IX in the next section in connection with determination of the total nuclear collision cross section in the target.

In the present calculation all nuclear scattering of protons below 20 MeV and all elastic scattering of neutrons above 15 MeV have been neglected. Inclusion of these processes would result in a small increase in the total damage energy cross section. In addition, the effect of Coulomb scattering of above-cutoff protons has been included only in terms of its effect on the proton trajectories, not in terms of kinetic energy transmitted to lattice nuclei. Preliminary estimates indicate that inclusion of damage energy contributions from above-cutoff proton Coulomb scattering may increase the damage energy cross section calculated here by perhaps 10 to 20%, and these scattering processes will be treated in future calculations. Finally, the effects of the subsequent decays which the radioactive spallation nuclei undergo have been neglected. Since virtually all these nuclei decay by electron or positron emission, the decays make no significant contribution to either the damage energy or light particle/nucleus production cross section.

IV. COMPARISON WITH NEUTRON DAMAGE EFFECTS

Of the many complex factors which determine the rate and nature of the radiation damage produced in a target bombarded by a beam of particles with a given energy spectrum, three which are strongly spectrum-dependent are the number of displacements per atom (dpa) produced by an average particle in the beam and the amount of transmutation-nucleus and of light-gas production (hydrogen and helium, which play important roles in embrittlement and in void formation) in relation to dpa. Since the dpa per damage-producing particle is generally assumed to be proportional to the damage energy cross section for the particle, it will be sufficient to use $\langle E_D \rangle$ for the purpose of comparing damage effects of various spectra.

TABLE IX

DAMAGE-RELATED SPECTRUM-AVERAGED CROSS SECTIONS FOR SEVERAL NEUTRON SPECTRA, AND THE CORRESPONDING CROSS SECTIONS CALCULATED HERE FOR 800-MeV PROTONS

Spectrum	σ_T (b)	$\sigma_{n,\alpha}$ (mb)	$\sigma_{n,p}$ (mb)	$\langle E_D \rangle$ (b-keV)	$\langle \bar{E}_D \rangle$ (b-keV)
HFIR	7.086	0.079	4.3	24.3	52.3
EBR II-7	5.587	0.032	1.8	32.4	44.7
EBR II-2	4.706	0.077	4.3	45.1	52.3
^{235}U	3.655	0.281	17.9	83.2	84.0
"14 MeV"	2.948	35.61	78.8	273	273
BENCH	5.156	9.26	24.7	99.9	130

Beam	σ_T (b)	σ_{He} (mb)	σ_p (mb)	$\langle E_D \rangle$ (b-keV)
800 MeV p	1.03 ^a 1.56 ^a	400 ^b	2580	330 ^a 350 ^a

^aThe top figure gives charged-particle results only, the bottom figure includes neutron effects with a geometrical factor of 0.5 cm.

^bThis figure combines ^3He and ^4He and adds a factor two.

The DON code has been used to calculate spectrum-averaged cross sections of several types for a number of neutron spectra, a few of which are shown in Table IX. HFIR is the neutron spectrum at the PTP location in the High Flux Isotope Reactor at ORNL; EBR II-2 and EBR II-7 refer to the neutron spectra at the midplanes of the second and seventh rows in the Experimental Breeder Reactor II core, respectively; ^{235}U is the spectrum of ^{235}U fission neutrons; "14 MeV" is an average for 13.5-15 MeV neutrons; and BENCH is a hypothetical fusion reactor first-wall spectrum based on the ORNL Benchmark Design. The spectrum-averaged cross sections given in the first three columns after the spectrum designation are the total neutron cross section σ_T , the total (n, α) cross section $\sigma_{n,\alpha}$, and the total (n,p) cross section $\sigma_{n,p}$.²⁰ Protons and alphas can also

be produced in reactions of the form (n,Xp) and (n,X α); but the cross sections for reactions of this type in copper are small in the energy region of interest, and the (n,p) and (n, α) cross sections shown may be considered effectively the total proton and alpha production cross sections for their respective spectra. In the next column is the damage energy cross section $\langle E_D \rangle$ for each spectrum normalized to the fast neutron flux above about 1 eV. For the neutron spectra shown this effectively normalizes the damage energy cross section to the full spectrum of damage producing neutrons, so that the relative sizes of the numbers in this column indicate the relative displacement-producing effectiveness of the various spectra. Since experimental results are often reported in terms of fluences above 0.1 MeV only, the last column gives a damage energy cross section $\langle \bar{E}_D \rangle$

TABLE X

CROSS-SECTION RATIOS OF DAMAGE RELEVANCE

Damage Source	$\{\sigma_{\text{He}}/\langle E_D \rangle\} \times 10^6$ (keV ⁻¹)	$\sigma_p/\sigma_{\text{He}}$	$\{\sigma_{\text{trans}}/\langle E_D \rangle\} \times 10^3$ (keV ⁻¹)
HFIR	3.24	54	0.18
EBR II-7	0.99	56	0.056
EBR II-2	1.70	56	0.098
²³⁵ U	3.38	64	0.22
"14-MeV"	130	2.2	2.75
BENCH	92.7	2.7	1.75
800-MeV p	1100 ^a	6.5	2.9

^aAssumes $\langle E_D \rangle = 350.5$ -keV.

"renormalized" to the neutron flux above 0.1 MeV. These renormalized cross sections when multiplied by fluences above 0.1 MeV yield the damage energy per atom generated in a target irradiated by the neutron source; but the relative sizes of these renormalized cross sections have no particular significance, and only the damage energy cross sections $\langle E_D \rangle$ normalized to the full damage-producing neutron flux will be considered below.

To permit easy comparison, the total cross section, total helium production cross section, total proton production cross section, and damage energy cross section calculated here for 800-MeV protons are shown in a separate section of Table IX. The total cross section and damage energy cross section are each shown two ways; first, ignoring the effects of the neutrons produced; and second, incorporating these effects assuming a geometrical factor 0.5 ca. The helium production cross section shown for an 800-MeV proton has been obtained by adding the calculated ³He and ⁴He cross sections, and then multiplying by two to approximately compensate for the known tendency of NMTC to underestimate helium production by about this amount. The cross section shown should therefore be considered only a rough estimate of the correct value. Neutron-produced contributions to proton and helium production have not been shown because they constitute only small corrections to the cross sections shown. The production cross section for all types of hydrogen is 10% larger than the proton production cross section shown.

The directly interpretable column in Table IX is that giving the damage energy cross sections $\langle E_D \rangle$ for each case. These cross sections show that one 800-MeV proton deposits as much damage energy in a thin copper target as 1.3 "14-MeV"-neutrons, 3.5 first-wall fusion neutrons, 4.2 ²³⁵U fission neutrons, .8 EBR II-2 neutrons, 11 EBR II-7 neutrons, or 14 FIR neutrons. To make comparisons with regard to light gas production it is necessary to consider certain ratios of the cross sections appearing in Table X, and two such ratios are given for each of the seven spectra in the first two columns of Table X. In the first column is shown the ratio of the helium production and damage energy cross sections. It is seen that the ratio of helium production to damage production for the fission spectra is about two orders of magnitude less than the ratio for the

"14-MeV" and BENCH spectra, while that for 800-MeV protons is one order of magnitude greater. The second column in Table X gives the ratio of proton to helium production for the various spectra. In this case it is seen that the ratios for the "14-MeV," BENCH, and 800-MeV proton cases are rather close to each other, and the ratios for the fission spectra are all about an order of magnitude higher. In comparing the ratios for 800-MeV protons with those for the neutron spectra it should be kept in mind that the production cross section for He is poorly known in the proton case. A decrease in the cross-section value used (here 0.4 b) would decrease the first-column entry and increase the second.

One final quantity which might be important in the radiation damage process is the ratio between the number of impurity nuclei introduced into the target material by nuclear transmutations and the number of displacements produced. This ratio will be proportional to the ratio of the total cross section for transmutations and the damage energy cross section, which is shown for each of the seven cases in the last column of Table X. Again it is seen that the 800-MeV proton, "14-MeV," and BENCH results are quite close to each other, and the four fission cases lie between one and two orders of magnitude lower. In calculating transmutation cross sections for the six neutron spectra (n,p), (n,α), and (n,2n) cross sections were taken into account. The (n,p) cross section constitutes almost the entire contribution to σ_{trans} for the four fission spectra, while the (n,2n)

cross section gives 80% and 85% of the contribution for the BENCH and "14-MeV" spectra, respectively. By reference to Table III one sees that the nuclei ^{62}Cu and ^{64}Cu which are obtained from natural copper by (n,2n) processes in neutron bombardment occur with relatively high probability in the 800-MeV proton case also. However, ^{59}Co , ^{61}Co , ^{63}Zn , and ^{65}Zn , which are obtained from ^{63}Cu and ^{65}Cu by (n, α) and (n,p) processes, are not among even the top twenty nuclides with highest production cross sections in the 800-MeV proton case (and in fact occupy positions 23, 43, 53, and 79, respectively). Thus even though the numbers of impurity nuclei per dpa will be approximately the same for the 800-MeV proton case as for the "14-MeV" and BENCH spectra, the variety of impurity nuclides produced is much greater for the proton case. No attempt has yet been made by the authors to determine what effect, if any, this difference in the types of nuclei produced may have in the total radiation damage process.

V. CONCLUSIONS

From the figures in Table X it appears likely that radiation damage effects due to 800-MeV protons incident on copper will be closer to those of "14-MeV"/BENCH-spectrum neutrons than either of these will be to the damage effects of any of the four fission sources. Also, as commented earlier, the proton damage effects are quite uniform over the 1-cm target thickness considered in the present calculation and probably would remain reasonably uniform over thicknesses two to three times as great. Consequently it is possible to obtain bulk damage effects in samples large enough for mechanical testing. According to the damage energy cross sections of Table IX, a 50- μA current of 800-MeV protons uniformly distributed over a target area of 1 cm^2 is equivalent in damage energy deposition to a BENCH-spectrum neutron flux of $10^{15}\text{ cm}^{-2}\text{ sec}^{-1}$. This is only 5% to 10% of the current ultimately expected in the 800-MeV proton beam of the Los Alamos Meson Physics Facility (LAMPF). No high-energy neutron source currently available comes as close as an order of magnitude to this equivalent number of BENCH-spectrum neutrons per second. Indeed, the primary limitation on damage rate by proton bombardment is imposed by target cooling requirements. For 50 $\mu\text{A}/\text{cm}^2$ about $1\text{ kW}/\text{cm}^3$ of heat energy must be dissipated. Probably about ten

times this volume heating rate, corresponding to a current density of $500\text{ }\mu\text{A}/\text{cm}^2$, could be handled without undue experimental difficulty in samples tens of mils thick. This produces a damage energy deposition rate about ten times that in a sample in the EBR II-2 position. These figures and the results shown in Table X suggest that for some time to come neutron damage simulation by high-current medium-energy proton accelerators such as that at LAMPF may provide one of the more useful and accurate ways of obtaining experimental information for large classes of materials concerning bulk damage to be expected in fusion spectrum situations. The damage rates achievable in moderately thick samples suggest certain fission-reactor-relevant damage studies can also be carried out advantageously by medium-energy proton bombardment; however, the poorer correspondence in light gas and transmutation nucleus production rates will require more extensive theoretical and experimental interpolation in this case.

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REFERENCES

1. W. A. Coleman, and T. W. Armstrong, Nucl. Sci. Eng. 43, 353 (1971); "The Nucleon-Meson Transport Code NMTC," ORNL-4606, Oak Ridge National Laboratory (October 1970). The version of NMTC used incorporates the MECC-2 intranuclear cascade code and the EVAP-4 evaporation code.
2. Philip A. Seeger, private communication.
3. J. Lindhard, V. Nielsen, and M. Scharff, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. 36, No. 10 (1968).
4. J. Lindhard, M. Scharff, and H. E. Schiøtt, *Ibid.*, 33, No. 14 (1963).
5. J. Lindhard, V. Nielsen, M. Scharff, and P. V. Thomsen, *Ibid.*, 33, No. 10 (1963).
6. D. M. Parkin, and A. N. Goland, "Calculation of Radiation Effects as a Function of Incident Neutron Spectrum," Rad. Effects (in press).
7. T. W. Armstrong, J. Geophys. Res. 74, 1351 (1969).
8. T. W. Armstrong, and B. L. Bishop, Radiat. Res. 47, 581 (1971).

9. T. W. Armstrong, K. G. Alsmiller, Jr., K. C. Chandler, and B. L. Bishop, Nucl. Sci. Eng. 49, 82 (1972).
10. H. W. Bertini, M. P. Guthrie, and A. H. Culkowski, "Nonelastic Interaction of Nucleons and π -mesons with Complex Nuclei Below 3 Gev," ORNL-TM-3148, Oak Ridge National Laboratory (1972).
11. For closely related calculations and methods see D. K. Brice, Rad. Effects 6, 77 (1970); J. Appl. Phys. 46, 3385 (1975); Proc. International Conference on Fundamental Aspects of Radiation Damage in Metals (October 1975), to be published; I. Manning, and G. P. Mueller, Computer Phys. Comm. 7, 85 (1974).
12. M. T. Robinson, "The Energy Dependence of Neutron Radiation Damage in Solids," B.N.E.S. Nuclear Fusion Reactors Conference at Culham Laboratory Proc. (September 1969), pp. 364-378.
13. See the third reference of No. 11 for a similar treatment.
14. J. F. Janni, "Calculations of Energy Loss, Range, Pathlength, Scattering, Multiple Scattering, and the Probability of Inelastic Nuclear Collisions for 0.1- to 1000-MeV Protons," report AFWL-TR-65-150, Air Force Weapons Laboratory, Kirtland Air Force Base, NM (1966).
15. M. T. Robinson, "The Production of Displaced Atoms in Solids," report AEKE-R7934, AERE Harwell, Oxfordshire, England (1975), p. 18.
16. J. Narayan, T. S. Noggle, and O. S. Oen, "Depth Distribution of Damage in Copper Irradiated with MeV He and Ni Ions," Proc. International Conference on Fundamental Aspects of Radiation Damage in Metals (October 1975), to be published.
17. M. T. Robinson, "The Theory of Defect Production," Ibid.
18. J. B. Roberto, J. Narayan, and M. J. Saltmarsh, "15 MeV Neutron Damage in Cu and Nb," Proc. International Conference on Radiation Effects and Tritium Technology for Fusion Reactors (October 1975), to be published.
19. J. B. Mitchell, R. A. Van Konynenburg, and D. M. Parkin, "DT Fusion Neutron Radiation Strengthening of Copper and Niobium," Ibid.
20. The two sets of cross sections shown for EBR II may be slightly low, because the calculated energy spectra used in their determination extended only to 10 MeV. However, the qualitative conclusions drawn are valid irrespective of this spectrum truncation.