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## Standard Practice for Investigating the Effects of Neutron Radiation Damage Using Charged-Particle Irradiation<sup>1</sup>

This standard is issued under the fixed designation E521; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon ( $\epsilon$ ) indicates an editorial change since the last revision or reapproval.

### INTRODUCTION

This practice is intended to provide the nuclear research community with recommended procedures for using charged-particle irradiation to investigate neutron radiation damage mechanisms as a surrogate for neutron irradiation. It recognizes the diversity of energetic-ion producing devices, the complexities in experimental procedures, and the difficulties in correlating the experimental results with those produced by reactor neutron irradiation. Such results may be used to estimate density changes and the changes in microstructure that would be caused by neutron irradiation. The information can also be useful in elucidating fundamental mechanisms of radiation damage in reactor materials.

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### 1. Scope

1.1 This practice provides guidance on performing charged-particle irradiations of metals and alloys, although many of the methods may also be applied to ceramic materials. It is generally confined to studies of microstructural and microchemical changes induced by ions of low-penetrating power that come to rest in the specimen. Density changes can be measured directly and changes in other properties can be inferred. This information can be used to estimate similar changes that would result from neutron irradiation. More generally, this information is of value in deducing the fundamental mechanisms of radiation damage for a wide range of materials and irradiation conditions.

1.2 Where it appears, the word “simulation” should be understood to imply an approximation of the relevant neutron irradiation environment for the purpose of elucidating damage mechanisms. The degree of conformity can range from poor to nearly exact. The intent is to produce a correspondence between one or more aspects of the neutron and ~~charged-particle~~ charged-particle irradiations such that fundamental relationships are established between irradiation or material parameters and the material response.

1.3 The practice appears as follows:

<sup>1</sup> This practice is under the jurisdiction of ASTM Committee E10 on Nuclear Technology and Applications and is the direct responsibility of Subcommittee E10.05 on Nuclear Radiation Metrology.

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1.4 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.5 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.*

1.6 *This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.*

## 2. Referenced Documents

### 2.1 ASTM Standards:<sup>2</sup>

[C859 Terminology Relating to Nuclear Materials](#)

[E170 Terminology Relating to Radiation Measurements and Dosimetry](#)

[E821 Practice for Measurement of Mechanical Properties During Charged-Particle Irradiation](#)

[E910 Test Method for Application and Analysis of Helium Accumulation Fluence Monitors for Reactor Vessel Surveillance](#)

[E942 Guide for Investigating the Effects of Helium in Irradiated Metals](#)

### 2.2 ICRU Documents:<sup>3</sup>

[ICRU 60 Fundamental Quantities and Units for Ionizing Radiation](#)

[ICRU 85a Fundamental Quantities and Units for Ionizing Radiation](#)

## 3. Terminology

### 3.1 Definitions of Terms Specific to This Standard:

3.1.1 Descriptions of relevant terms are found in Terminology [C859](#) and Terminology [E170](#).

### 3.2 Definitions:

<https://standards.iteh.ai/catalog/standards/sist/cffid4789-4c06-4883-98cd-1b1da392bf49/astm-e521-23>

3.2.1 *damage energy,  $n$ — $T_{dam}$* —that portion of the energy lost by an ion moving through a solid that is transferred as kinetic energy to atoms of the medium; strictly speaking, the energy transfer in a single encounter must exceed *the  $T_d$  energy required to displace an atom from its lattice site.*

3.2.2 *displacement,  $n$ — $n$* —the process of dislodging an atom from its normal site in the lattice.

3.2.3 *path length,  $n$ — $n$* —the total length of path measured along the actual path of the particle.

3.2.4 *penetration depth,  $n$ — $n$* —a projection of the range along the normal to the entry face of the target.

3.2.5 *projected range,  $n$ — $n$* —the projection of the range along the direction of the incidence ion prior to entering the target.

3.2.6 *range,  $n$ — $n$* —the distance from the point of entry at the surface of the target to the point at which the particle comes to rest.

3.2.7 *stopping power (or stopping cross section),  $n$ — $n$* —the energy lost per unit path length due to a particular process; usually expressed in differential form as  $-dE/dx$ .

<sup>2</sup> For referenced ASTM standards, visit the ASTM website, [www.astm.org](http://www.astm.org), or contact ASTM Customer Service at [service@astm.org](mailto:service@astm.org). For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

<sup>3</sup> ICRU Report 60 has been superseded by ICRU Report 85a on Fundamental Quantities and Units for Ionizing Radiation, October 2011. Both of these documents are available from International Commission on Radiation Units and Measurements (ICRU), 7910 Woodmont Ave., Suite 800, Bethesda, MD 20814.

### 3.2.7.1 *Discussion*—

The stopping power is commonly divided into an electronic and a nuclear component (ICRU).

3.2.8 *straggling*, *straggling—n*—the statistical fluctuation due to atomic or electronic scattering of some quantity such as particle range or particle energy at a given depth.

### 3.3 *Symbols*:

3.3.1  $A_1$ ,  $Z_1$ —the atomic weight and the number of the bombarding ion.

$A_2$ ,  $Z_2$ —the atomic weight and number of the atoms of the medium undergoing irradiation.

*depa*—damage energy per atom; a unit of radiation exposure. It can be expressed as the product of  $\sigma_{de}^-$  and the fluence.

*dpa*—displacements per atom; a unit of radiation exposure giving the mean number of times an atom is displaced from its lattice site. It can be expressed as the product of  $\sigma_d^-$  and the fluence.

*heavy ion*—used here to denote an ion of mass  $>4$ .

*light ion*—an arbitrary designation used here for convenience to denote an ion of mass  $\leq 4$ .

$T_d$ —an effective value of the deposited energy required to displace an atom from its lattice site. Usual unit is eV.

$\sigma_d(E)$ —an energy-dependent displacement cross section;  $\sigma_d^-$  denotes a spectrum-averaged value. Usual unit is barns.

$\sigma_{de}(E)$ —an energy-dependent damage energy cross section;  $\sigma_{de}^-$  denotes a spectrum-averaged value. Usual unit is barns-eV or barns-keV.

## 4. Significance and Use

4.1 A characteristic advantage of charged-particle irradiation experiments is the precise, ~~individual,~~ individual control over most of the important irradiation conditions such as dose, dose rate, temperature, and quantity of gases present. Additional attributes are the lack of induced radioactivation of specimens and, in general, a substantial compression of irradiation time, from years to hours, to achieve comparable damage as measured in displacements per atom (dpa). An important application of such experiments is the investigation of radiation effects that may be obtained in occur in materials exposed to environments which do not currently exist, such as in first wall materials used in fusion reactors.

4.2 The primary shortcoming of ion bombardments stems from the damage rate, or temperature dependences of the microstructural evolutionary processes in complex alloys, or both. It cannot be assumed that the time scale for damage evolution can be comparably compressed for all processes by increasing the displacement rate, even with a corresponding shift in irradiation temperature. In addition, the confinement of damage production to a thin layer just (often  $\sim 1 \mu\text{m}$ ) below the irradiated surface can present substantial complications. It must be emphasized, therefore, that these experiments and this practice are intended for research purposes and not for the certification or the qualification of materials.

4.3 This practice relates to the generation of irradiation-induced changes in the microstructure of metals and alloys using charged particles. The investigation of mechanical behavior using charged particles is covered in Practice E821.

## 5. Apparatus

5.1 *Accelerator*—The major item is the accelerator, which in size and complexity dwarfs any associated equipment. Therefore, it is most likely that irradiations will be performed at a limited number of sites where accelerators are available (a 1-MeV electron microscope may also be considered an accelerator).

5.2 *Fixtures*, for holding specimens during irradiation are generally custom-made as are devices to measure and control particle energy, particle ~~flux (fluence rate),~~ fluence rate (recommended terminology for the deprecated term “flux”), and specimen temperature. Decisions regarding apparatus are therefore left to individual workers with the request that accurate data on the performance of their equipment be reported with their results.

## 6. Composition of Specimen

6.1 An elemental analysis of stock from which specimens are fabricated should be known. The manufacturer’s heat number and analysis are usually sufficient in the case of ~~commercially~~ commercially produced metals. Additional analysis should be performed after other steps in the experimental procedure if there is cause to believe that the composition of the specimen may have been altered. It is desirable that uncertainties in the analyses be stated and that an atomic basis be reported in addition to a weight basis.

## **7. Preirradiation Heat Treatment of Specimen**

7.1 Temperature and time of heat treatments should be well controlled and reported. This applies to intermediate anneals during fabrication, especially if a metal specimen is to be irradiated in the cold-worked condition, and it also applies to operations where specimens are bonded to metal holders by diffusion or by brazing. The cooling rate between annealing steps and between the final annealing temperature and room temperature should also be controlled and reported.

7.2 The environment of the specimen during heat treatment should be reported. This includes description of container, measure of vacuum, presence of gases (flowing or steady), and the presence of impurity absorbers such as metal sponge. Any discoloration of specimens following an anneal should be reported.

7.3 High-temperature annealing of metals and alloys from Groups IV, V, and VI frequently results in changes, both positive and negative, in their interstitial impurity content. Since the impurity content may have a significant influence on void formation, an analysis of the specimen or of a companion piece prior to irradiation should be performed. Other situations, such as selective vaporization of alloy constituents during annealing, would also require a final analysis.

7.4 The need for care with regard to alterations in composition is magnified by the nature of the specimens. They are usually very thin with a high exposed surface-to-volume ratio. Information is obtained from regions whose distance from the surface may be small relative to atomic diffusion distances.

## **8. Plastic Deformation of Specimen**

8.1 When plastic deformation is a variable in radiation damage, care must be taken in the geometrical measurements used to compute the degree of deformation. The variations in dimensions of the larger piece from which specimens are cut should be measured and reported to such a precision that a standard deviation in the degree of plastic deformation can be assigned to the specimens. A measuring device more accurate and precise than the common hand micrometer will probably be necessary due to the thinness of specimens commonly irradiated.

8.2 The term *cold-worked* should not stand alone as a description of state of deformation. Every effort should be made to characterize completely the deformation. The parameters which should be stated are: (1) deformation process (for example, simple tension or compression, swaging, rolling, rolling with applied tension); (2) total extent of deformation, expressed in terms of the principal orthogonal natural strain components ( $\epsilon_1, \epsilon_2, \epsilon_3$ ) or the geometric shape changes that will allow the reader to compute the strains; (3) procedure used to reach the total strain level (for example, number of rolling passes and reductions in each); (4) strain rate; and (5) deformation temperature, including an estimate of temperature changes caused by adiabatic work.

8.2.1 Many commonly used deformation processes (for example, rolling and swaging) tend to be nonhomogeneous. In such cases the strain for each pass can be best stated by the dimensions in the principal working directions before and after each pass. The strain rate can then be specified sufficiently by stating the deformation time of each pass.

## **9. Preirradiation Metallography of Specimen**

9.1 A general examination by light microscopy and transmission-electron microscopy should be performed on the specimen in the condition in which it will be irradiated. In some cases, this means that the examination should be done on specimens that were mounted for irradiation and then unmounted without being irradiated. The microstructure should be described in terms of grain size, phases, precipitates, dislocations, and inclusions.

9.2 A section of a representative specimen cut parallel to the particle beam should be examined by light microscopy. Attention should be devoted to the microstructure within a distance from the incident surface equal to the range of the particle, as well as to the flatness of the surface.

## **10. Surface Condition of Specimen**

10.1 The surface of the specimen should be clean and flat. Details of its preparation should be reported. Electropolishing of metallic specimens is a convenient way of achieving these objectives in a single operation. The possibility that hydrogen is

absorbed by the specimen during electropolishing should be investigated by analyses of polished and nonpolished specimens. Deviations in the surface from the perfect-planar condition should not exceed, in dimension perpendicular to the plane, 10 % of the expected particle range in the specimen.

10.2 The specimen may be irradiated in a mechanically polished condition provided damage produced by polishing does not extend into the region of postirradiation examination.

## 11. Dimension of Specimen Parallel to Particle Beam

11.1 Specimens without support should be thick enough to resist deformation during handling. If a disk having a diameter of 3 mm is used, its thickness should be greater than 0.1 mm.

11.2 Supported specimens may be considerably thinner than unsupported specimens. The minimum thickness should be at least fourfold greater than the distance below any surface from which significant amounts of radiation-produced defects could escape. This distance can sometimes be observed as a void-free zone near the free surface of an irradiated specimen.

## 12. Helium

### 12.1 *Injection:*

12.1.1 Alpha-particle irradiation is frequently used to inject helium into specimens to simulate the production of helium during neutron irradiations where helium is produced by transmutation reactions. Helium injection may be completed before particle irradiation begins. It may also proceed incrementally during interruptions in the particle irradiation or it may proceed simultaneously with particle irradiation. The last case is the most desirable as it gives the closest simulation to neutron irradiation. Some techniques for introducing helium are set forth in Guide E942.

12.1.2 The influence of implantation temperature on how helium is distributed in the material (that is, whether helium is dispersed in the lattice, in small clusters, in bubbles, etc.) is known to be important. The consequences of the choice of injection temperature on the simulation should be evaluated and reported.

### 12.2 *Analysis and Distribution:*

12.2.1 Analysis of the concentration of helium injected into the specimens should be performed by mass spectrometry. Using this technique, the helium content is determined by vaporizing a helium-containing specimen under vacuum, adding a known quantity of  $^3\text{He}$ , and measuring the  $^4\text{He}/^3\text{He}$  ratio. This information, along with the specimen weight, will give the average helium content in the specimen. The low-level  $^2\text{He}$  addition is obtained by successive expansion through calibrated volumes. The mass spectrometer is repeatedly calibrated for mass fractionation during each series of runs by analyzing known mixtures of  $^3\text{He}$  and  $^4\text{He}$ . Other methods of measurement, such as the nondestructive  $\alpha$ - $\alpha$  scattering technique, may be employed, but their results should be correlated with mass spectrometric results to ensure accuracy. employed. Refer to Test Method E910 and Guide E942 for additional details.

12.2.2 In many experiments, attempts are made to achieve uniformity of helium content within the damage region by varying the incident energy of the alpha-particle beam and by avoiding fluence variations on the specimen surface. The success of these attempts should be measured by analyzing separate sections of the specimen for helium. It may be necessary to use several companion specimens for this purpose. Variation of helium concentration through the thickness of the specimen as well as variations across the specimen can also be nondestructively measured with the  $\alpha$ - $\alpha$  scattering technique.

12.3 *Alpha-Particle Damage*—Alpha-particle irradiation produces some displacement damage in the specimen. This damage, which changes as the specimen is heated for irradiation by other particles, may influence the radiation effects subsequently produced. Therefore, in those cases where helium injection precedes the particle irradiation, a specimen should be brought to the irradiation temperature in the same manner as if it were going to be irradiated and then examined by transmission-electron microscopy at ambient temperature to characterize the microstructure.

## 13. Irradiation Procedure

13.1 *Quality of Vacuum*—Contamination of the specimen surface by oxidation or deposition of foreign matter and diffusion of impurities into the specimen must be avoided. A vacuum of 133  $\mu\text{Pa}$  ( $10^{-6}$  torr) or smaller should be maintained during irradiation

for most nonreactive metals. High-temperature irradiation of metals from Groups IV, V, or VI should be done in a vacuum of 1.33  $\mu\text{Pa}$  ( $10^{-8}$  torr) or smaller. Oil-diffusion pumps should be cold-trapped to restrict the passage of hydrocarbons into the target chamber and beam tube. The target chamber should be baked periodically or as needed to limit the buildup of contaminants on the walls of the chamber and that a cold-trapped, liquid nitrogen or similarly cold anti-contamination device be installed near the target to trap as many contaminants as possible. The visual appearance of the specimen after irradiation and the vacuum maintained during irradiation should be reported.

### 13.2 *Specimen Temperature:*

13.2.1 The temperature of the specimen should not be allowed to vary by more than  $\pm 10^\circ\text{C}$ ;  $\pm 10^\circ\text{C}$ . It should be controlled, measured, and recorded continuously during irradiation. Infrared sensors offer a direct method of measuring actual temperature of the specimen surface. If thermocouples are used, they should be placed directly on the specimen to avoid temperature gradients and interfaces between the thermocouple and the specimen, which will produce a difference between the thermocouple reading and the actual temperature of the specimen volume being irradiated. A thermocouple should not be exposed to the particle beam because spurious signals may be generated.

13.2.2 Beam heating should be minimized relative to nonbeam heating to minimize temperature fluctuations of the specimen due to fluctuations in beam ~~flux (fluence rate)~~ fluence rate and energy. If a direct measurement of specimen temperature during irradiation cannot be made, then the specimen temperature should be calculated. Details of the calculation should be fully reported.

13.3 *Choice of Particle*—Since the accelerated particles usually come to rest within the specimen, the possibility of significant alterations in specimen composition exists with concomitant effects on radiation damage. If metallic ions are used, they should be of the major constituents of the specimen. Electron irradiation poses no problems in this regard.

### 13.4 *Choice of Particle Energy:*

13.4.1 Three criteria should be considered in the choice of particle energy:

(1) The range of the particle should be large enough to ensure that the region to be examined possesses a ~~preirradiation~~ pre-irradiation microstructure that is unperturbed by its proximity to the surface.

(2) The point defect concentration during irradiation in the observed volume should not differ substantially from that expected of irradiated volumes located far from free surfaces.

(3) The energy deposition gradient parallel to the beam across the volume chosen for observation should be small over a distance that is large compared to typical diffusion distances of defects at the temperature of interest. The best measure of surface influence is the observation of denuded zones for the microstructural feature of interest. The width of denuded zones for voids can be significantly larger or smaller than those observed for dislocations. The volume of the specimen to be examined should lie well beyond the denuded zone because steep concentration gradients of point defects may exist on the boundary of such zones. Gradients in the deposited energy can be reduced by rocking the specimen (varying the angle between the beam and the specimen surface), but local time-dependent ~~flux~~ fluence rate variations will exist.

13.4.2 The nominal energy of the accelerated particle should be verified periodically by calibration experiments. These experiments should be reported and an uncertainty assigned to the energy.

### 13.5 *Purity of Beam:*

13.5.1 The use of a bending magnet is an effective way of selecting a particular ion for transit through the beam tube to the specimen. However, it is possible that the selected ions will interact with foreign atoms in the beam tube, causing foreign atoms to strike the specimen also and altering the charge and energy on the selected ion.

13.5.2 A good vacuum in the beam tube will eliminate the significance of these effects, and therefore this vacuum should be monitored during irradiation. A discoloration of the specimen surface could indicate a problem in this regard even though a satisfactory vacuum exists in the vicinity of the specimen.

### 13.6 *Flux (fluence rate): Fluence Rate:*

13.6.1 The particle ~~flux (fluence rate)~~ fluence rate on the specimen should be recorded continuously during irradiation and integrated with time to give the fluence. This is particularly important since most accelerators do not produce a constant ~~flux~~. Fluence rate. Fluence rate and fluence should be reported as particles/ $\text{m}^2\cdot\text{s}$  and particles/ $\text{m}^2$ . For the case where the particle comes

to rest within the specimen, the specimen holder assembly should be designed as a Faraday cup. The flux-fluence rate measured this way should be checked with a true Faraday cup that can be moved in and out of the beam. If the particles are transmitted through the specimen, a Faraday cup can be positioned on the exit side for flux-fluence rate measurement. Variations in flux-fluence rate during the irradiation should be reported.

13.6.2 It is desirable that the flux-fluence rate be the same everywhere on the specimen surface. The actual flux-fluence rate variation in a plane parallel to the specimen surface should be measured and considered when interpreting results of postirradiation examination. A beam profile monitor is recommended for this purpose. It is possible to mitigate the effects of a spatially nonhomogeneous beam by moving the beam over the surface of the specimen during irradiation. A defocused beam should be used; the maximum translation should be less than the beam half-width. The uniformity or nonuniformity of the beam should be reported with the method used for this purpose.

13.6.3 Rastering (periodic scanning) of a focused beam over the specimen will subject the specimen to periodic local flux-fluence rate variations. It is recommended that a rastered beam be avoided for the simulation of a constant neutron flux-fluence rate, although it may be appropriate for the simulation of a pulsed neutron flux-fluence rate. Radiation-induced defect structures that evolve under such pulsed conditions can differ substantially from those that evolve in a constant flux-fluence rate. Recent work has identified conditions in which significant microstructural differences are observed when a rastered beam is used **(1, 2)**<sup>4</sup>. It should be noted that pulsed operation is an inherent characteristic of many accelerators.

## 14. Damage Calculations

14.1 *Scope*—This section covers methods and problems of determining displacement rates for ions and electrons in the energy ranges most likely to be employed in simulations of fission and fusion reactor radiation effects. These are 0.1 to 70 MeV for ions and 0.2 to 10 MeV for electrons, although not all energies within these ranges are treated with equal precision. To provide the basis for subsequent descriptions of neutron-charged particle correlations, the calculation of displacement rates in neutron irradiations is also treated.

14.2 *Energy Dissipation by Neutrons and Charged Particles*—See **Appendix X1**.

14.3 *Particle Ranges*—Ions suffer negligible deflections in encounters with electrons; hence, if electron losses dominate, differences between range, projected range, and path length will be small. Furthermore, energy dissipation in this case is by a large number of low-energy-exchange events, so range straggling will be small and, at a given depth (except near end of range), energy straggling will be small. These conditions apply to light ions for energies down to the tens of keV range, but only at much higher energies for heavy ions such as nickel.

### 14.3.1 Light Ions:

14.3.1.1 Stopping powers of light ions are easiest to calculate in the range of several MeV to several tens of MeV, but these calculations cannot be done accurately from first principles **(3-5)**. At lower energies, heavy reliance must be placed on the few experimental measurements of stopping powers. Several tabulations of stopping powers and the path lengths deduced from them exist **(3-6-710)**. A modern Monte Carlo code, SRIM, can also be easily used to compute the required ranges and stopping powers **(811)**.

14.3.1.2 Although the work by Janni **(69)** appears to be the most comprehensive one for protons, experimental range data **(912)** have been produced that are in disagreement with his tables for 1-MeV protons incident on steel. In view of the better agreement of the tables of Williamson et al. **(47)** with these data, it was recommended **(1013)** that the latter tables be used for the path length of protons in iron and nickel and their alloys. Ranges can be obtained from these path length values by subtracting a correction for multiple scattering as given by Janni, but this correction is only -2.2% at 0.1 MeV, decreasing to -0.8% at 5 MeV for protons incident on iron. Ranges for iron should be valid also for steels and nickel-base alloys to within the accuracy of the tables (several percent). The referenced tables should be consulted for data on proton ranges in other metals (the distinction between path length and range is generally ignored) and for deuteron and alpha ranges **(710)**. Range estimates can conveniently be made for deuterons and alphas in terms of those for protons for energies at which the stopping power is primarily electronic by employing the following equations:

$$R^{\alpha}(E) \cong R^p(E/4) \quad (1)$$

$$R^d(E) \cong 2 R^p(E/2) \quad (2)$$

<sup>4</sup> The boldface numbers in parentheses refer to the list of references appended to this practice.

These approximations agree with tabulated values to within better than 5 % for alpha energies >8 MeV and deuteron energies >2 MeV, the accuracy increasing with increasing energy.

14.3.2 *Heavy Ions:*

14.3.2.1 Heavy ions suffer increasing range straggling as the energy is decreased—the spread in range is a large fraction of the mean range at 1 MeV. This corresponds to an increasing fraction of energy lost as kinetic energy imparted to atoms (nuclear stopping) as opposed to excitation and ionization of electrons (electronic stopping).

14.3.2.2 Ranges of heavy ions in the low MeV range cannot be calculated with high accuracy. A semi-empirical tabulation of ranges by Northcliffe and Schilling is available (36), and a more recent tabulation of range distributions and stopping powers is contained in a series of books edited by Ziegler and coworkers (710). Note that the ranges in Ref (36) (actually path lengths) have been corrected for nuclear stopping, whereas their tabulated stopping powers are for electronic stopping only.

14.3.2.3 Ranges are generally tabulated as areal densities, for example, mg/cm<sup>2</sup>; as such they are invariant to changes in mass density. In particular, they apply to material containing voids. The linear range is obtained by dividing the areal density by the mass density—the latter must of course be the actual density, including a correction for void volume if present. An increase in range straggling and energy straggling is caused by the production of voids during an irradiation (H14).

14.3.2.4 Ranges can be computed with a code developed by Johnson and Gibbons (H215). It is included as a subroutine in the E-DEP-1 Code (see 14.4.3.1). It permits evaluations of projected ranges and range straggling as well. More recently, the SRIM code (811) has been used for such calculations.

14.3.3 *Electrons:*

14.3.3.1 Electrons are subject to many large-angle scattering events; hence range straggling is severe. In radiation damage studies, however, the primary concern is with the passage of electrons through relatively thin targets in which the fractional energy loss is small. This loss can be estimated for many purposes using the following general prescription. The principal loss mechanisms are ionization and radiation. If  $x$  is the projected range and  $N$  and  $Z$  are the atomic density and atomic number of the target, respectively:

$$dE/dx |_{ion} \propto NZ \tag{3}$$

$$dE/dx |_{rad} \propto NZ^2 E \tag{4}$$

for  $E > 1$  MeV. Hence, given values for some reference material, energy dissipation for any other material can be estimated. A convenient reference material is lead, in which both mechanisms contribute approximately equally at 10 MeV:

$$dE/dx |_{ion} \cong dE/dx |_{rad} \cong 16 \text{ MeV/cm} \tag{5}$$

(or 1.6 keV/μm) 10 MeV in Pb

Using this relation to evaluate the proportionality factors for a second material with atomic number  $Z_2$  and atomic mass  $A_2$  yields:

$$dE/dx |_{ion} \cong 0.357 p_0 Z_2 / A_2 \text{ keV/}\mu\text{m} \tag{6}$$

or:

$$3.57 p_0 Z_2 / A_2 \text{ MeV/cm}$$

$$dE/dx |_{rad} \cong 0.000435 E(\text{MeV}) p_0 Z_2^2 / A_2 \text{ keV/}\mu\text{m}$$

or:

$$0.00435 E(\text{MeV}) p_0 Z_2^2 / A_2 \text{ MeV/cm} \tag{7}$$

where  $p_0$  is the mass density. For example, these relations give:

$$dE/dx |_{ion} \cong 13 \text{ MeV/cm}$$

and:

$$dE/dx |_{rad} \cong 4 \text{ MeV/cm}$$

for 10-MeV electrons in iron. For 1-MeV electrons in iron, this procedure overestimates the radiation loss by a factor of 3 but at this energy the ionization loss accounts for over 90 % of the energy loss.

14.4 *Damage Energy Calculations:*



14.4.1 *Damage Energy*—A necessary (but not sufficient) condition for consistency between displacement damage estimates for neutrons and charged particles is that the same energy partition model be used in calculating the damage energy. The currently recommended model ([1013](#), [1316](#), [1417](#)) is due to Lindhard et al. ([1518](#)); the expression for the damage energy  $T_{\text{dam}}(T)$  lost by a knock-on of initial kinetic energy  $T$  is:

$$T_{\text{dam}} = T[1 + kg(\epsilon)]^{-1} \quad (8)$$

$$k = 0.1337 Z_1^{2/3} A_1^{-1/2}$$

$$= T/(0.08693 Z_1^{2/3})$$

$$T_{\text{dam}}(T) = T[1 + kg(\epsilon)]^{-1} \quad (8)$$

When the incident ion and the lattice ion are the same:

$$k = 0.1337 Z_1^{2/3} A_1^{-1/2}$$

$$\epsilon = T/(0.08693 Z_1^{2/3})(keV)$$

Following Robinson and coworkers ([1619](#), [1720](#)):

$$g(\epsilon) = \epsilon + 0.40244\epsilon^{3/4} + 3.4008\epsilon^{1/6} \quad (9)$$

$$\epsilon = \frac{A_2 T}{(A_1 + A_2)} \frac{a}{Z_1 Z_2 e^2} \quad (10)$$

$$a = a_o \left( \frac{9\pi^2}{128} \right)^{1/2} (Z_1^{2/3} + Z_2^{2/3})^{-1/2} \quad (11)$$

The general expression for  $\epsilon$ , when the incident and lattice atoms are different, is given by:

$$\epsilon = \frac{A_2 T}{(A_1 + A_2)} \frac{a}{Z_1 Z_2 e^2} \quad (10)$$

$$a = a_o \left( \frac{9\pi^2}{128} \right)^{1/2} (Z_1^{2/3} + Z_2^{2/3})^{-1/2} \quad (11)$$

where  $a_o$  is the Bohr radius ( $5.292 \times 10^{-9}$  cm),  $e$  is the electronic charge ( $4.803 \times 10^{-10}$  statcoulomb), and the subscripts 1 and 2 on the atomic numbers ( $Z$ ) and atomic masses ( $A$ ) denote the incident ion and the target atoms, respectively. These units require that the kinetic energy,  $T$ , in Eq 10 be expressed in ergs.

14.4.1.1 Strictly speaking, this energy partitioning model expression for the energy partitioning model, as derived by Robinson, can only be applied to monatomic systems, that is, and was developed for the cases where  $Z_1 = Z_2$ . However, it can reasonably be applied as long as these two values are sufficiently close ([1619](#)). In the case of alloy (polyatomic) targets, an effective  $Z$  should be calculated by weighting the alloy constituents by their respective atomic fractions. For polyatomic lattice materials where the atoms have significant differences in the  $Z$ , this use of an effective  $Z$  has limitations ([21](#)). In addition, the Lindhard model is limited to energies  $T$  less than about  $25 \cdot Z_1^{4/3} \cdot A_1$  (in keV) ([1619](#)).

#### 14.4.2 Neutrons:

14.4.2.1 The calculation of damage energy for neutron irradiations is most conveniently expressed in terms of an energy-dependent damage energy cross section,  $\sigma_{de}(E)(E)$ . This expresses the damage energy per atom per unit neutron fluence; a convenient unit is eV-barns. In calculating this cross section, all possible reactions that can transfer sufficient energy to an atom of the medium to displace it must be considered. These include elastic scattering, inelastic scattering, neutron multiplication reactions [for example, (n,2n)], charged-particle-out reactions [for example, (n,p)], (for example, (n,2n)), charged-particle production reactions (for example, (n,p)), and absorption reactions (n, $\gamma$ ). Most of the necessary data are included in the ENDF/BENDF/B-VIII.0 files ([1822](#)), and it is recommended that these be used in damage calculations.

14.4.2.2 The treatment of the kinematics for these reactions has been documented ([19-23-2125](#)); the result is a cross section  $d\sigma(T,E)$  for the production, by all possible reactions, of a primary knock-on atom (PKA) of energy  $T$  by a neutron of energy  $E$ . The damage energy cross section is then simply the integral of the product of this primary cross section and the damage energy,  $T_{\text{dam}}$ , associated with a PKA of energy  $T$ :

$$\sigma_{de}(E) = \int_0^{T_m} T_{\text{dam}} [d\sigma(T,E)/dT] dT \quad (\text{eV} - \text{barns}) \quad (12)$$

The upper limit of the integral,  $T_m$ , is the maximum possible PKA energy, in the absence of charged particle emission, it emission. For elastic scattering reactions, the conservation of energy and momentum imply that the maximum transferred energy results from a head-on elastic collision and is given by:

$$T_m = 4A_1A_2/(A_1 + A_2)^2 E \quad (13)$$

$$T_m = 4A_1^2/(A_1 + 1)^2 E \quad (13)$$

where the atomic weight is expressed in terms of neutron masses, as in ENDF/BENDF/B-6 notation. Higher values of  $T_m$  are possible in some charged-particle-out reactions that are exoergic. The lower limit in Eq 12 was sometimes assumed to be zero since, even when the PKA energy is less than  $T_{df}$ , an effective displacement energy, the non-ionizing portion of the PKA energy is deposited in the material lattice as phonon energy, while not resulting in a lattice atom displacement and the production of a Frenkel pair. Note that the integral in Eq 12 is over the PKA energy while  $T_{df}$  when based on the Kinchin-Pease and NRT formulations, refers to the non-ionizing damage energy that corresponds to the energy of this recoil atom. When the incident neutron energy,  $E_i$ , exceeds several keV, the difference between using  $T_{df}$  and 0 in this equation is small.

14.4.2.3 To determine the damage energy density in a neutron-irradiated material, the neutron flux-spectrum-fluence rate spectrum  $\phi(E)$  must be known. The damage energy deposition per atom (depa) per second is then:

$$\text{depa/s} = \int_0^\infty \phi(E) \sigma_{de}(E) dE \quad (14)$$

This can be converted to damage energy per cubic centimeter per second by multiplying by  $N$ , the atom density. The cumulative damage energy density is obtained by integrating over the irradiation time.

14.4.2.4 Since, for most reactor spectra, the damage energy contributed by neutrons of energy less than a few keV is negligible, the depa for neutron irradiations is generally independent of the value used for  $T_{df}$  (see further discussion under 13.6.214.4.4.1).

#### 14.4.3 Heavy Ions:

14.4.3.1 In general, the damage energy depends on the ion energy so it will vary with penetration. A simple computer code, E-DEP-1 (2226), was developed and extensively applied for calculating damage energy versus depth distributions for heavy ions. It made the simplifying assumption of approximating energy straggling by using the range straggling theory of Lindhard et al. (2327). Also implicit is the additional assumption that the ranges of knock-on atoms are negligible; that is, all damage energy is deposited in the immediate vicinity of the point at which the incident ion produces the knock-on atom (energy transport is neglected). Beeler (2428) has performed computer experiments and Winterbon (2529) has made analytical calculations to estimate the effect of this assumption on the shape of the damage energy-depth profile. The effect is not large for experiments that effectively integrate over macroscopic intervals (for example, 50 nm) of the profile. The more modern Monte Carlo code SRIM (811, 2630, 2731) is now most commonly used to perform these calculations. The use of SRIM permits more sophisticated analyses to be performed than does EDEP-1. SRIM is relatively fast and can be used for both light- and heavy-ion irradiations as long as nuclear reactions are not involved.

14.4.3.2 The damage-energy density increases with depth, reaches a peak, and then drops rapidly to zero. In the vicinity of the peak, the uncertainty in the E-DEP-1 calculation must be assumed large—perhaps 25 to 50 % (4013). Nearer the specimen surface where the gradient and damage energy is less, the uncertainty is perhaps 20 %. The uncertainty in SRIM calculations may be lower. Measurements of observed damage versus depth are highly recommended if the intent is to make damage observations in the peak damage region.

14.4.3.3 In applying E-DEP-1, the user has the option of describing electronic stopping of the incident ion using the expression for  $k$  given by Lindhard et al. (2327), or reading in some other value.  $k$  is the proportionality factor between the electronic stopping power and the ion velocity. SRIM includes a more modern description of electronic stopping. Lindhard et al. gives the approximate expression:

$$k = 0.0793 Z_1^{1/6} (Z_1 Z_2 / Z)^{1/2} A_2 / A_0^{3/2} \quad (15)$$

in which:

$$Z^2 = Z_1^{3/2} + Z_2^{3/2}, A_0 = A_1 A_2 / (A_1 + A_2) \quad (16)$$

It is suggested that better  $k$  values may be determined directly from the tabulated stopping powers of Northcliffe and Schilling (36).

#### 14.4.4 Light Ions:

14.4.4.1 Damage energy estimates for light ions at low energies can be made in a more straightforward manner. The mean energy,  $E_x$ , at depth  $x$  is first determined from tables as follows. Let  $E_0$  be the incident ion energy and  $R(E)$  the mean range of an ion of energy  $E$ . Assume range and energy straggling are negligible. Then the residual range of an ion at  $x$  is  $R(E_x) = R(E_0) - x$ . Given  $E_0$  and  $x$ , one can find  $R(E_0)$  in the range-energy tables, calculate  $R(E_x)$ , and thus determine  $E_x$  from the tables. A knowledge of  $E_x$  permits application of the Rutherford scattering cross section,  $d\sigma_R(T, E_x)$ , which gives the approximate number of knock-ons in the interval  $dT$  at knock-on energy  $T$  that is produced by an ion of energy  $E_x$  (2832):

$$d\sigma_R(T, E_x) = (B\gamma^2/E_x)(dT/T^2) \quad (17)$$

where:

$$B = 4\pi a_0^2 E_R^2 (A_1/A_2) Z_1^2 Z_2^2,$$

$\gamma_1 Z_1$  = effective charge of the moving ion,  
 $a_0$  = 0.053 nm, and  
 $E_R$  = 13.6 eV.

A convenient expression for  $\gamma$  given by Bichsel (2933) is  $\gamma = 1 - \exp(-1.316 y + 0.1112 y^2 - 0.0650 y^3)$ ;  $y = 100\beta/Z_1^{2/3}$  where  $\beta \ll 1$  is the ratio of the particle velocity to that of light. Expressed as a function of particle energy,  $y = (4.63/Z_1^{2/3}) [E_x(\text{MeV})/A_1]^{1/2}$ . The damage energy cross section is given by integrating over the product of the number of events producing a knock-on of energy  $T$  [ $d\sigma_R(T, E_x)$ ] and the damage energy associated with the knock-on,  $T_{\text{dam}}$ :

$$\sigma_{de}(E_x) = (B\gamma^2/E_x) \int_{T_d}^{T_m} T_{\text{dam}} (dT/T^2) \quad (18)$$

$$\sigma_{de}(E_x) = (B\gamma^2/E_x) \int_{T_{\text{dam}}^{-1}(T_d)}^{T_m} \frac{T_{\text{dam}}(T)}{T^2} dT \quad (18)$$

Unlike Eq 12, the lower limit of this integral which includes an explicit form for the cross section is the mean energy required to displace an atom, that is, to deliver a damage energy of  $T_d$ . From Eq 8, this corresponds to a recoil energy,  $T$ , such that  $T_{\text{dam}}(T) = T_d$  and thus, the lower integration bound is given by the inverse function,  $T_{\text{dam}}^{-1}(T_d)$ .  $T_m$  is the upper limit and represents the maximum possible energy transferred to an atom through an elastic scattering and is given by:

$$T_m = 4A_1 A_2 / (A_1 + A_2)^2 E_x \quad (19)$$

$$T_m = 4A_1 A_2 / (A_1 + A_2)^2 E_x \quad (19)$$

Then  $\text{depa/s}$  is the product of the particle flux-fluence rate  $\phi$  and  $\sigma_{de}$ . If the atom density is  $N$  and the irradiation time is  $t$ , the damage energy density ( $\text{eV/cm}^3$ ) is given by  $\phi t N \sigma_{de}$ .

14.4.4.2 The Rutherford scattering cross section describes only coulomb scattering. Another source of elastic scattering for light ions above several MeV is nuclear potential scattering. Large-angle coulomb scattering is rare and hence large-angle elastic scattering will be dominated by potential scattering above several MeV, as discussed by Logan et al. (3034) for niobium. To calculate correctly the elastic scattering contribution to the displacement cross section, experimental data on angular differential cross sections or optical model code computations of these cross sections must be used. The results for medium  $Z$  materials are generally lower than obtained, assuming coulomb scattering. However, in the same energy range, nonelastic scattering begins to become significant. Rigorous calculations of this contribution have not yet been made, although the approximate method used by Logan et al. is probably adequate. It appears that nonelastic scattering will become dominant with increasing energy and will generally more than offset the decrease in the elastic contribution relative to coulomb scattering. That is, Eq 2 may significantly underestimate the damage energy cross section for light ions above  $\sim 10$  MeV.

14.4.5 *Electrons*—The concept of damage-energy density is not particularly helpful in electron irradiations except for very high electron energies because mean knock-on energies generally do not greatly exceed displacement thresholds. However, the damage energy can be estimated from Oen's tables (3135) as  $T_{\text{dam}} \cong \frac{2}{3} T_d \sigma_d$ , where  $\sigma_d$  is Oen's displacement cross section. Note that Oen used the energy-partition sharp threshold displacement model of original Kinchin and Pease (36) rather than that of Lindhard et al. or Lindhard or NRT threshold treatment (18).

## 14.5 Conversion of Damage Energy to DPA:

### 14.5.1 Model:

14.5.1.1 A secondary displacement model describes the number of displacements  $N_{\text{dcl}}$  produced in a cascade initiated by a PKA of kinetic energy  $T$ . The simplified model recommended here is based on Ref (4619) and has been adopted by both the IAEA (4316) and researchers in the U.S. (4013, 4417) (for iron, nickel, and their alloys):

$$\begin{aligned}
 N_d &= 0 & T < T_d \\
 N_d &= 1 & T_d \leq T < 2T_d\beta \\
 N_d &= \beta T_{\text{dam}}/2T_d & T \geq 2T_d\beta \quad (20)
 \end{aligned}$$

The previously recommended values for iron, steel, and nickel-base alloys are  $\beta = 0.8$  and  $T_{\text{dcl}} = 40$  eV, or  $N_{\text{dcl}} = 10 T_{\text{dam}}$ , if  $T_{\text{dam}}$  is expressed in keV. While the value assigned to the effective displacement energy,  $T_d$ , is somewhat arbitrary, it is most important that a specific secondary displacement model be used for the purpose of standardization; hence the model presented in Eq 20 is recommended. There is some error incurred in using Eq 20 due to the neglect of inelastic energy losses at very low energies. Robinson and Oen have discussed this in detail and provide an expression for a simple correction factor (3237).

14.5.1.2 The actual displacement energy depends on the direction of ejection of the atom (3338) (see Appendix X1). The value of  $T_{\text{dcl}}$  used in Eq 20 should represent an average overall ejection direction taken over all of the ejection directions. Sufficient data to permit calculation of  $T_{\text{dcl}}$  exist for only a few metals. In any event, the value of 40 eV recommended for steels is based largely on computer simulation of low-energy cascades, rather than directly on displacement threshold measurements. The point here is that there is no basis for assigning overly precise  $T_{\text{dcl}}$  values for various metals. In order to foster uniformity in displacement calculations, a list of recommended  $T_{\text{dcl}}$  values is given in Table 1, along with some measured threshold values. The  $T_{\text{dcl}}$  values are rounded to emphasize their approximate nature. The recommended values are generally consistent with molecular dynamics simulations that have investigated the directional dependence of the displacement threshold in a number of materials (3338). The values obtained for iron using molecular dynamics simulations are in generally good agreement with an extensive investigation using *ab initio* calculations to determine the angular dependence of the displacement threshold (3439). For those metals for which Lucasson (see Table 1) gives average values, the agreement is with 10 % except for Cr, Ni, and Nb. The value for Cr was set equal to that recommended for Fe and Ni (Lucasson gives 60 eV for Cr and 33 eV for Ni), since it is generally of concern only as a component of stainless steel. The value for Nb (Lucasson gives 78 eV) was set equal to that for Mo, consistent with some existing displacement calculations; there is little evidence for using different values.

#### 14.5.2 Neutrons:

14.5.2.1 The calculation of a damage energy cross section,  $\sigma_{de}$  (see 14.4), is simply converted to the calculation of a displacement cross section,  $\sigma_d$ , by replacing  $T_{\text{dam}}$  with  $N_{\text{dcl}}$  in Eq 13.  $\sigma_d$ , usually expressed in barns, represents the number of displacements per atom (dpa) per unit neutron fluence. For practical purposes, the difference in the form of  $N_{\text{dcl}}(T_{\text{dam}})$  between  $T_{\text{dcl}}$  and  $2T_{\text{dcl}}/\beta$  can be ignored and one can write:

**TABLE 1 Recommended Values of the Effective Displacement Energy for Use in Displacement Calculations**

Metal	$T^{\text{min}}$ (eV) <sup>A</sup>	$T_{\text{dcl}}$ (eV)
Al	16	25
Ti	19	30
V	—	40
Cr	28 <sup>B</sup>	40
Mn	—	40
Fe	20 <sup>B</sup>	40
Co	22	40
Ni	23	40
Cu	19	30
Zr	21	40
Nb	36 <sup>B</sup>	60
Mo	33	60
Ta	34	90
W	40	90
Pb	14	25

<sup>A</sup> See review by P. Lucasson in *Proceedings of International Conference on Fundamental Aspects of Radiation Damage in Metals*, Gatlinburg, Tenn., TN, October 1975.

<sup>B</sup> An effective threshold measured in a polycrystalline specimen.