Designation: E693 – 01 (Reapproved 2007)

Standard Practice for Characterizing Neutron Exposures in Iron and Low Alloy Steels in Terms of Displacements Per Atom (DPA), E 706(ID)[1]

This standard is issued under the fixed designation E693; 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 (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice describes a standard procedure for characterizing neutron irradiations of iron (and low alloy steels) in terms of the exposure index displacements per atom (dpa) for iron.

1.2 Although the general procedures of this practice apply to any material for which a displacement cross section $\sigma_d(E)$ is known (see Practice E521), this practice is written specifically for iron.

1.3 It is assumed that the displacement cross section for iron is an adequate approximation for calculating displacements in steels that are mostly iron (95 to 100 %) in radiation fields for which secondary damage processes are not important.

1.4 Procedures analogous to this one can be formulated for calculating dpa in charged particle irradiations. (See Practice E521.)

1.5 The application of this practice requires knowledge of the total neutron fluence and flux spectrum. Refer to Practice E521 for determining these quantities.

1.6 The correlation of radiation effects data is beyond the scope of this practice.

1.7 *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 and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*[2]

E170 Terminology Relating to Radiation Measurements and Dosimetry

E521 Practice for Neutron Radiation Damage Simulation by Charged-Particle Irradiation

E560 Practice for Extrapolating Reactor Vessel Surveillance Dosimetry Results, E 706(IC)[3]

E821 Practice for Measurement of Mechanical Properties During Charged-Particle Irradiation

E853 Practice for Analysis and Interpretation of Light-Water Reactor Surveillance Results, E706(IA)

3. Terminology

3.1 Definitions for terms used in this practice can be found in Terminology E170.

4. Significance and Use

4.1 A pressure vessel surveillance program requires a methodology for relating radiation-induced changes in materials exposed in accelerated surveillance locations to the condition of the pressure vessel (see Practices E560 and E853). An important consideration is that the irradiation exposures be expressed in a unit that is physically related to the damage mechanisms.

4.2 A major source of neutron radiation damage in metals is the displacement of atoms from their normal lattice sites. Hence, an appropriate damage exposure index is the number of times, on the average, that an atom has been displaced during an irradiation. This can be expressed as the total number of displaced atoms per unit volume, per unit mass, or per atom of the material. Displacements per atom is the most common way of expresssing this quantity. The number of dpa associated with a particular irradiation depends on the amount of energy deposited in the material by the neutrons, and hence, depends on the neutron spectrum. (For a more extended discussion, see Practice E521.)

4.3 No simple correspondence exists in general between dpa and a particular change in a material property. A reasonable starting point, however, for relative correlations of property changes produced in different neutron spectra is the dpa value associated with each environment. That is, the dpa values

[1] 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.

Current edition approved June 1, 2007. Published July 2007. Originally approved in 1979. Last previous edition approved in 2001 as E693 – 01(2007). DOI: 10.1520/E0693-01R07.

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

[3] Withdrawn. The last approved version of this historical standard is referenced on www.astm.org.

themselves provide a spectrum-sensitive index that may be a useful correlation parameter, or some function of the dpa values may affect correlation.

4.4 Since dpa is a construct that depends on a model of the neutron interaction processes in the material lattice, as well as the cross section (probability) for each of these processes, the value of dpa would be different if improved models or cross sections are used. The calculated dpa cross section for ferritic iron, as given in this practice, is determined by the procedure given in 6.3. A considerable body of irradiated materials data has been reported using dpa cross sections based on the iron ENDF/B-IV (**1, 2**)[4] cross section. The recent changes in the iron cross section (**3**), the recommendation to use the updated iron cross sections in radiation transport calculations of pressure vessel spectra (**4**), and the recent availability of ENDF/B-VI iron dpa cross section calculations (**1, 2, 5**) have resulted in the update of the recommended dpa cross section to reflect the ENDF/B-VI cross sections (**1**). Although the ENDF/B-VI based dpa cross section differs from the previously recommended ENDF/B-IV dpa cross section (**1**) by about 60 % in the energy region around 10 keV, by about 10 % for energies between 100 keV and 2 MeV, and by a factor of 4 near 1 keV due to the opening of reaction channels in the cross section, the integral iron dpa values are much less sensitive to the change in cross sections. The update from ENDF/B-IV to ENDF/B-VI dpa rates when applied to the H. B. Robinson-2 pressurized water reactor results in "up to ~4 % higher dpa rates in the region close to the pressure vessel outer surface" and in "slightly lower dpa rates ... close to the pressure vessel inner wall" (**6, 7**). Thus the update of the recommended dpa exposure parameter to reflect an iron cross section consistent with that used in the current radiation transport calculations is "not expected to introduce a bias in embrittlement data bases" (**6**) based on the change in the dpa cross section. Table 1 presents a comparison of the previous edition (Practice E693-94) and currently recommended dpa estimates for several neutron spectra.

5. Procedure

5.1 The displacement rate at time t is calculated as follows:

$$\text{dpa/s} = \int_0^\infty \sigma_d(E)\phi(E,t)\,dE \tag{1}$$

where:

$\sigma_d(E)$ = the displacement cross section for a particular material, and

$\phi(E,t)\,dE$ = the fluence rate of neutrons in the energy interval E to $E + dE$.

5.2 The exposure index, dpa, is then the time integrated value of the displacement rate, calculated as follows:

$$\text{dpa} = \int_0^{t_r} \phi_{\text{tot}}(t) \int_0^\infty \sigma_d(E)\psi(E,t)\,dE\,dt \tag{2}$$

where:

$\phi_{\text{tot}}(t)$ = the time dependent fluence rate intensity, and

$\psi(E,t)$ = the fluence rate spectrum normalized to give unit integral fluence rate at any time when integrated over energy.

5.2.1 If the fluence rate spectrum is constant over the duration, t_r, of the irradiation, then:

$$\text{dpa} = \phi_{\text{tot}} t_r \int_0^\infty \sigma_d(E)\psi(E)\,dE = \phi_{\text{tot}} t_r \bar{\sigma}_d \tag{3}$$

where $\bar{\sigma}_d$ = the spectrum-average displacement cross section.

5.3 It is assumed for purposes of this practice that the fluence $\phi_{\text{tot}} t_r$ and the spectrum $\psi(E)$ are known.

6. Calculation

6.1 The integral can be evaluated by a simple numerical integration as follows:

$$\int_0^\infty \sigma_d(E)\phi(E)\,dE = \sum_{i=1}^{N} (\sigma_d)_i \phi_i \Delta E_i \tag{4}$$

[4] The boldface numbers in parentheses refer to the list of references appended to this practice.

TABLE 1 Changes in Spectrum-Integrated dpa for Benchmark Neutron Spectra

Neutron Spectrum	Spectrum-averaged dpa cross section (barns)[A]		
	"Old" ENDF/B-IV-based E693 response	"Current" ENDF/B-VI-based E693 response	Difference ([Current - Old]/Old) (%)
ENDF/B-VI ^{235}U Thermal Fission **(1, 2)**	875.55	858.54	–1.9
Materials Dosimetry Reference Facility (MDRF) **(8)**	345.03	343.58	–0.42
CFRMF **(9, 10)**	382.94	387.08	1.08
Intermediate-energy Standard Neutron Field (ISNF) **(10, 11)**	483.63	480.00	–0.75
Arkansas Nuclear ONE-1 (ANO) Cavity **(12, 13)**	134.40	139.44	3.75
ORNL Poolside Facility (PSF) T/4 position **(12, 14)**	242.14	238.33	–1.57
Oak Ridge Research Reactor (ORR) **(10)**	291.68	288.86	–0.97
Yayoi **(10)**	613.12	609.03	–0.67
BIGTEN **(10, 15)**	334.98	341.25	1.87
H.B. Robinson-2, in the vessel wall, close to the inner surface **(6, 7)**	219.43	218.81	–0.28
H.B. Robinson-2, ~¼ T vessel wall **(6, 7)**	245.17	249.24	1.66
H.B. Robinson-2, ~¾ T vessel wall **(6, 7)**	203.68	211.23	3.71

[A] The spectrum-average dpa values in this table were computed using Eq 11 in a 640 SAND-II energy group representation and a lower integration bound of $E_o = 10^{-10}$ MeV.

NOTE 1—Table 1 is included to illustrate the effect on the dpa cross sections resulting from the change from the ENDF/B-IV to ENDF/B-VI cross sections. The spectrum-average cross section values given are not recommended for other uses because of their sensitivity to the assumed spectrum representations and the lower energy integration limit.

where $(\sigma_d)_i$ and ϕ_i are grouped-averaged values over the interval $E_i < E < E_{i+1}$, and ΔE_i is the width of the interval and is given by $E_{i+1} - E_i$.

6.2 The only computational problem, then, is to obtain $\sigma_d(E)$ and $\phi(E)$ in the same group structure. $\sigma_d(E)$ is available (**16**) in the SAND-II group structure (included here as Table 2), which is as fine or finer than the group structure in which $\phi(E)$ is generally available. Hence the problem is to collapse $\sigma_d(E)$ to match the $\phi(E)$ group structure.

6.2.1 If the $\phi(E)$ group structure is sufficiently fine, a simple group averaging is sufficient:

$$(\sigma_d)_i = \frac{1}{\Delta E_i} \sum_{k=1}^{M_i} (\sigma_d)_{ik} \Delta E_{ik} \tag{5}$$

where M_i is the number of groups in $\sigma_d E$ between E_i and E_{i+1}, and the $\Delta E_{ik} \equiv E_{ik+1} - E_{ik}$ are the group widths.

6.2.1.1 If the ΔE_{ik} are constant (as above 1 MeV in Table 2), this becomes a simple average of the M_i groups in ΔE_i as follows:

$$(\sigma_d)_i = \frac{1}{M_i} \sum_{k=1}^{M_i} (\sigma_d)_{ik} \tag{6}$$

6.2.2 For a coarse group representation of $\phi(E)$, the group averages of $\sigma_d(E)$ should be weighted averages, unless such weighting has been shown to have negligible effects. The ideal weighting function is, of course, the actual spectrum $\phi(E)$. For light-water reactor applications, a generalized spectrum is often used consisting of a fission spectrum plus a low energy $1/E$ tail. Let the weighting spectrum be designated by $W(E)$. Then the recommended form and energy regimes are as follows:

$$W(E) = C_1/E \qquad \text{E} < 0.82 \text{ MeV} \tag{7}$$

$$= C_2 E^{1/2} e^{-E/1.4} \qquad \text{E} \geq 0.82 \text{ MeV}$$

The constants C_1 and C_2 are arbitrary.

The group averages are then computed from the following equation:

$$(\sigma_d)_i = \frac{\sum_{k=1}^{M_i} (\sigma_d)_{ik} W(\hat{E}_{ik}) \Delta E_{ik}}{\sum_{k=1}^{M_i} W(\hat{E}_{ik}) \Delta E_{ik}} \tag{8}$$

where $\hat{E}_{ik}$ = the average energy of the k^{th} group, or

$$\hat{E}_{ik} \equiv (E_{ik+1} + E_{ik})/2 \tag{9}$$

NOTE 1—This standard does not address the adequacy of the neutron group structure used for the representation and calculation of the energy dependent variations in the neutron spectrum. At positions within thick pressure vessels, Eq 8 may not provide correct results unless the energy groups, indexed by the letter i, are chosen to be adequate for representing the neutron spectrum variations.

6.2.3 It may be that the group structure of $\phi(E)$ is not a subset of the group structure of $\sigma_d(E)$; that is, none of the values of E_{ik} coincide with E_i or E_{i+1}, or both. This should pose no problem because the $\sigma_d(E)$ group structure is sufficiently fine that accurate interpolation is easily accomplished.

6.3 The recommended displacement cross section for iron $\sigma_d(E)$, is given as a function of energy in Table 2. The energy values chosen for the table entries are those of the SAND-II energy group structure (**17**). The table is a listing of energies and corresponding displacement cross sections. A graphical display of the displacement cross sections as a function of energy appears in Fig. 1. This damage energy to displacement conversion procedure is consistent with Practices E521 and E821 recommendations on the treatment of radiation damage by charged particles. The values of the displacement cross section are based on ENDF/B-VI (revision 5) cross sections (**1, 2**) as processed into dpa cross sections with the NJOY-97 code (**18**) using the Robinson analytic representation (**19**) of the Lindhard model of energy partition between atoms and electrons (**20**) and the Norgett-Robinson-Torrens (NRT) recommended conversion of damage energy to displacements (**21**) with an effective displacement threshold energy of E_d=40 eV and an atomic scattering correction factor of β=0.8. The NRT displacement equation defines the number of displacements, N_d, corresponding to a given damage energy, T_d, through the equation

$$N_d(T_d) = \begin{bmatrix} 0 & T_d < E_d \\ 1 & E_d \leq T_d < 2\,E_d/\beta \\ \dfrac{\beta T_d}{2E_d} & 2E_d/\beta \leq T_d < \infty \end{bmatrix} \tag{10}$$

NOTE 2—The iron dpa cross section combines dpa from the individual ENDF/B-VI iron isotopic evaluations using the natural iron isotopic abundance values from Ref. (**22**). The isotopic cross sections and relative abundances used were:

26-Fe-54, Mat = 2625, Rev. 5, tape 140; rel. abundance = 5.9 %
26-Fe-56, Mat = 2631, Rev. 1, tape 123; rel. abundance = 91.72 %
26-Fe-57, Mat = 2634, Rev. 1, tape 123; rel. abundance = 2.1 %
26-Fe-58, Mat = 2637, Rev. 5, tape 140; rel. abundance = 0.28 %

NOTE 3—Version 97.45 of the NJOY97 code used in this analysis was modified to implement the NRT displacement threshold model.

6.4 A single calculation suffices, of course, to characterize a given spectrum in terms of the spectrum-averaged displacement cross section $\bar{\sigma}_d$.

6.4.1 The quantity $\bar{\sigma}_d$ is a good measure of spectrum hardness if the thermal-to-fast ratio is not large. However, a modified $\bar{\sigma}_d$ can be used with any thermal-to-fast ratio, if it is assumed that displacements are caused predominantly by neutrons of energies greater than E_o. Then one can define $\bar{\sigma}_d(E > E_o)$ by the following equation:

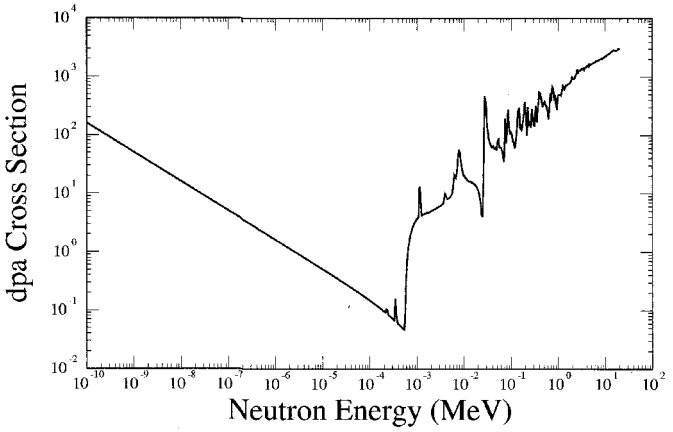

FIG. 1 ENDF/B-VI-based Iron Displacement Cross Section

$$\bar{\sigma}_d(E > E_0) = \frac{\int_{E_o}^{\infty} \sigma_d(E)\phi(E)dE}{\int_{E_o}^{\infty} \phi(E)\,dE} \quad (11)$$

and

$$\text{dpa/s} \cong \bar{\sigma}_d(E > E_o) \times \phi(E > E_o) \quad (12)$$

A reasonable value for E_o is 0.01 MeV. The quantity $\bar{\sigma}_d$ ($E >$ 0.01 MeV) is then a good index of spectrum hardness irrespective of the thermal-to-fast ratio.

7. Precision and Accuracy

7.1 *Precision*—The energy group structure selected to perform the integral in 6.1 should be selected such that the integral of the dpa exposure parameter over the neutron spectrum is within 1 % of that obtained when the complete 640-group SAND-II energy structure is used to represent the energy dependence of the dpa exposure parameter and the energy-dependent structure of the neutron spectrum. The precision in the spectrum-averaged dpa is dominated by the precision in the neutron spectrum characterization, including its representation of the fine energy structure.

7.2 *Accuracy*:

7.2.1 *Absolute Accuracy*—The absolute accuracy of the dpa calculation is not important when dpa is used as an exposure unit or correlation parameter for neutron irradiations, so long as a standard practice is used by all laboratories in calculating dpa. The absolute uncertainty is estimated to be 40 % or more when applied to a light water reactor spectrum (less in a softer spectrum). The major sources of error are the fluence spectrum, the reaction cross sections used in calculating $\sigma_d(E)$, the Lindhard model for the partition of energy between atoms and electrons, and the conversion of deposited energy to displacements.

7.2.2 *Relative Accuracy*—The relative accuracy of dpa calculations for different environments depends on the energy dependence of $\sigma_d(E)$ and on the relative accuracy of fluence-spectrum determinations. The covariance matrix for the iron dpa cross section is not available at present, although covariance matrices for the individual File 3 nuclear reaction cross sections which contribute to the dpa can be found in File 33 of the ENDF/B-VI cross section evaluations (**1**). For a discussion of the effect of the energy dependence of $\sigma_d(E)$ on the relative accuracy of the dpa calculation see Ref **23** and Practice E521. Losses in the relative accuracy of the dpa calculation due to this effect are estimated to be less than 10 % for most reactor spectra (**23**). The relative accuracy of the fluence-spectrum determination depends on the method of determination. (For recommended methods see E706, Matrix Standard.) Any uncertainty in the total fluence is, of course, reflected directly in the dpa calculation (see 5.2.1).

NOTE 4—Measurement uncertainty is described by a precision-and-bias statement in this standard. Another acceptable approach is to use Type A and B uncertainty components (**24, 25**). This Type A/B uncertainty specification is now used in International Organization for Standardization (ISO) standards and this approach can be expected to play a more prominent role in future uncertainty analyses.

8. Damage Correlation

8.1 This practice is concerned with standardizing a radiation exposure unit. It is concerned only secondarily with the correlation of damage produced in different environments. As stated in 4.1, the dpa is a logical first step in attempting to correlate displacement damage. Active research programs on improving the damage correlation methodology are in progress, and recent results (**26**) indicate that dpa can, in some cases, produce improved damage correlation when compared to fast neutron fluence. Because many past data correlations have been based on "fast fluence" ($E > 1$ MeV), this quantity should also be given, along with the dpa value, when expressing irradiation exposures. (For a general discussion of the damage correlation problem, see Ref **27**.)

9. Keywords

9.1 atomic displacements; cross section; irradiation; materials damage; neutron; steel

TABLE 2 ENDF/B-VI-based Iron Displacement Cross Section

Bin	Eng[A] (MeV)	σ_d(barns)	Bin	Eng[A] (MeV)	σ_d(barns)	Bin	Eng[A] (MeV)	σ_d(barns)
1	0.100E-09	158.3543	2	0.1050E-09	154.6209	3	0.110E-09	151.1395
4	0.1150E-09	147.8895	5	0.120E-09	144.1054	6	0.1275E-09	139.9202
7	0.1350E-09	136.0860	8	0.1425E-09	132.5445	9	0.150E-09	128.7502
10	0.160E-09	124.7860	11	0.170E-09	121.1728	12	0.180E-09	117.8527
13	0.190E-09	114.8137	14	0.200E-09	111.9561	15	0.210E-09	109.3199
16	0.220E-09	106.8646	17	0.230E-09	104.5694	18	0.240E-09	101.8930
19	0.2550E-09	98.93331	20	0.270E-09	96.65981	21	0.280E-09	94.12717
22	0.300E-09	91.05218	23	0.320E-09	88.24872	24	0.340E-09	85.68787
25	0.360E-09	83.33912	26	0.380E-09	81.17265	27	0.400E-09	78.92472
28	0.4250E-09	76.63646	29	0.450E-09	74.53734	30	0.4750E-09	72.59930
31	0.500E-09	70.81827	32	0.5250E-09	69.14790	33	0.550E-09	67.59222
34	0.5750E-09	66.13822	35	0.600E-09	64.64189	36	0.630E-09	63.12039
37	0.660E-09	61.70157	38	0.690E-09	60.37332	39	0.720E-09	58.92732
40	0.760E-09	57.39681	41	0.800E-09	55.97892	42	0.840E-09	54.65984
43	0.880E-09	53.43220	44	0.920E-09	52.28703	45	0.960E-09	51.21545
46	0.100E-08	50.07727	47	0.1050E-08	48.89598	48	0.110E-08	47.79609
49	0.1150E-08	46.76870	50	0.120E-08	45.57125	51	0.1275E-08	44.25006
52	0.1350E-08	43.03653	53	0.1425E-08	41.91761	54	0.150E-08	40.71708
55	0.160E-08	39.46333	56	0.170E-08	38.32018	57	0.180E-08	37.26968
58	0.190E-08	36.30967	59	0.200E-08	35.40710	60	0.210E-08	34.57391
61	0.220E-08	33.79705	62	0.230E-08	33.06956	63	0.240E-08	32.22424
64	0.2550E-08	31.28942	65	0.270E-08	30.57002	66	0.280E-08	29.76999