**Lattice Displacement Calculations and
Comparisons for Different Irradiation Facilities**

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MASTER

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FOR DIFFERENT IRRADIATION FACILITIES

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ABSTRACT

Descriptions of lattice displacement parameters are given, and methods for calculating displacement rates are described. Procedures are given for comparing displacement data from different irradiation facilities and effective damage fluence is defined. Values for effective graphite displacement cross sections and neutron fluxes are given for several irradiation facilities.

Key words: radiation damage, cross sections, graphite, in-pile tests, calculations, neutron flux, neutron spectra, HTGR.

INTRODUCTION

The mechanical and physical properties of all materials are altered by exposure to nuclear radiation. These property changes are usually degrading for most applications, and the irradiation damage is a major consideration in the design of nuclear systems. The mechanisms by which the damage occurs are varied and complex, but the damage mechanisms can be categorized by the initiating reactions. For example, the irradiation induced swelling of stainless steels, and the irradiation induced drift in thermocouples result from neutron induced isotopic transmutation reactions in the materials. The irradiation induced swelling in graphite, however, results from atomic lattice displacements caused primarily by neutron scattering reactions with carbon atoms.

The magnitude and the rate of irradiation damage for a specific material in a particular irradiation facility are functions of both the nuclear properties of the material and the neutronic characteristics of the facility. For this reason, comparisons of irradiation damage data from different facilities must involve both the material properties and the neutronic characteristics of the facility. Previous attempts to compare irradiation damage solely on the basis of some arbitrary neutronics

parameter (i.e., damage flux) were inaccurate and misleading. This memo identifies the factors involved in quantifying the displacement type of irradiation damage, and describes the procedures to be used for comparison of displacement damage data from different irradiation facilities. Graphite displacement damage is calculated for illustrative purposes, but the same methods can be applied to calculate displacement damage for any material.

DISPLACEMENT CROSS SECTIONS

The neutron induced lattice displacement rate in a material depends on the probability of a neutron reaction occurring, $\sigma_s(E)$, and the number of lattice displacements resulting from each reaction, $p(E)$. Therefore, a displacement cross section can be defined as:

$$\sigma_D(E) = \sigma_s(E) p(E) ,$$

where

$\sigma_D(E)$ = the displacement cross section; the displacement rate per unit neutron flux of energy E ,

$\sigma_s(E)$ = the neutron reaction cross section,

$p(E)$ = the displacement weighing function.

The displacement cross section is a material dependent parameter. Neutron reaction cross sections are available from sources such as ENDF/B libraries.¹ The displacement weighing functions are derived from physics considerations of atomic interactions in matter. The displacement weighing function most widely used for interpretation of graphite irradiation results was developed by Thompson and Wright.² Values of the scattering cross section and Thompson and Wright weighing function for graphite are summarized in Table 1. The displacement cross section for graphite is plotted versus energy in Fig. 1.

¹ENDF is the Evaluated Nuclear Data File and is the national reference set of evaluated cross section data.

²M. W. Thompson and S. B. Wright, "A New Damage Function for Predicting the Effect of Reactor Irradiation on Graphite in Different Neutron Spectra," *J. Nucl. Mater.* 16, 146-154 (1965).

Table 1. Group-averaged values of the graphite scattering cross section and the Thompson and Wright displacement weighing function

Neutron energy group	Upper energy (MeV)	ENDF-IV elastic scattering cross section for graphite (barns)	Thompson and Wright displacement weighing function
1	14.9	0.771	548.4
2	13.5	0.785	540.6
3	12.2	0.842	532.7
4	11.1	0.673	524.7
5	10.0	0.665	516.5
6	9.05	0.773	508.2
7	8.19	1.43	499.8
8	7.41	0.740	491.5
9	6.70	0.969	482.9
10	6.07	0.924	474.1
11	5.49	1.12	465.3
12	4.97	1.41	456.3
13	4.49	1.95	447.2
14	4.07	2.15	437.6
15	3.68	2.57	428.2
16	3.33	1.80	418.7
17	3.01	2.21	409.1
18	2.73	1.65	399.4
19	2.47	1.60	389.6
20	2.23	1.90	379.7
21	2.02	1.73	369.6
22	1.83	1.85	359.4
23	1.65	1.97	349.1
24	1.50	2.10	338.7
25	1.35	2.23	328.2
26	1.22	2.35	317.6
27	1.11	2.49	306.9
28	1.00	2.62	296.1
29	0.907	2.75	285.2
30	0.821	2.87	274.2
31	0.743	2.99	262.9
32	0.672	3.11	251.5
33	0.608	3.22	240.5
34	0.550	3.32	229.2
35	0.498	3.43	218.1
36	0.450	3.52	207.3
37	0.408	3.62	196.7
38	0.369	3.70	186.3
39	0.334	3.78	176.1
40	0.302	3.86	166.2

Table 1 (continued)

Neutron energy group	Upper energy (keV)	ENDF-IV elastic scattering cross section for graphite (barns)	Thompson and Wright displace- ment weighting function
41	273.0	3.93	156.5
42	247.0	4.00	147.0
43	223.0	4.06	137.8
44	202.0	4.12	128.8
45	183.0	4.17	120.0
46	166.0	4.22	111.5
47	150.0	4.26	103.2
48	136.0	4.30	95.2
49	123.0	4.34	87.4
50	111.0	4.40	74.8
51	86.5	4.47	61.2
52	67.4	4.53	49.7
53	52.5	4.57	40.2
54	40.9	4.61	32.3
55	31.8	4.63	25.9
56	24.8	4.65	20.7
57	19.3	4.67	16.5
58	15.0	4.68	13.1
59	11.7	4.69	10.3
60	9.12	4.70	8.0
61	7.10	4.71	6.2
62	5.53	4.71	4.8
63	4.31	4.71	3.7
64	3.35	4.72	2.9
65	2.61	4.72	2.3
66	2.03	4.72	1.8
67	1.58	4.72	1.4
68	1.23	4.72	1.1
69	0.961	4.72	0.8
70	0.749	4.73	0.6
71	0.583	4.73	0.5
72	0.454	4.73	0.4
73	0.353	4.73	0.3
74	0.275	4.73	0.2
75	0.214	4.73	0.1

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Fig. 1. Graphite displacement cross section.

DISPLACEMENT RATE

Each position in an irradiation facility has a unique time varying energy dependent neutron flux, $\phi(\bar{r}, E, t)$. The displacement rate for some material at each position can be expressed as:

$$D(\bar{r}, t) = \int_0^{\infty} \sigma_D(E) \phi(\bar{r}, E, t) dE ,$$

where

$D(\bar{r}, t)$ = the displacement rate per target atom at position $\bar{r}$ and time t .

The average displacement rate for an irradiation interval of duration T is then:

$$D(\bar{r}) = 1/T \int_0^T D(\bar{r}, t) dt .$$

If the energy dependence and magnitude of the neutron flux does not change during the irradiation, then $\phi(\bar{r}, E, t) = \phi(\bar{r}, E)$ and $D(\bar{r}) = D(\bar{r}, t)$, or

$$D(\bar{r}) = \int_0^{\infty} \sigma_D(E) \phi(\bar{r}, E) dE$$

or more simply

$$D = \int_0^{\infty} \sigma_D(E) \phi(E) dE .$$

EFFECTIVE DISPLACEMENT CROSS SECTIONS AND FLUX

Although the displacement rate, D , characterizes an irradiation position, effective cross sections and damage fluxes are sometimes convenient. The effective displacement cross section is defined by:

$$\bar{\sigma}_D(E_L) = \frac{\int_0^{\infty} \sigma_D(E) \phi(E) dE}{\int_{E_L}^{\infty} \phi(E) dE} = \frac{D}{\bar{\phi}(E_L)} ,$$

where

$\bar{\sigma}_D(E_L)$ = the effective displacement cross section for cutoff energy E_L ,

D = displacement rate per target atom,

$\bar{\phi}(E_L)$ = the integral neutron flux above the cutoff energy E_L ,
or the damage flux above E_L .

Note that

$$\bar{\sigma}_D(E_L) \bar{\phi}(E_L) = D \equiv \int_0^{\infty} \sigma_D(E) \phi(E) dE$$

is satisfied regardless of the energy E_L . Values of neutron fluxes and effective displacement cross sections for graphite are given in Table 2 for various reactor facilities and neutron energy spectra.

A special case arises when the neutron fission spectrum, $\chi(E)$, is used for the flux. In this case, a fission spectrum average displacement cross section, $\bar{\sigma}_x$, is obtained:

$$\bar{\sigma}_x = \frac{\int_0^{\infty} \sigma_D(E) \chi(E) dE}{\int_0^{\infty} \chi(E) dE}$$

This cross section is used as a comparative standard in ref. 3.

INTERCOMPARISON OF DISPLACEMENT DATA FROM DIFFERENT IRRADIATION FACILITIES

Some basis is frequently needed to facilitate comparisons of irradiation damage from different facilities. The most physically significant characteristics to compare would be the displacement rates for the facilities and the total displacements for a particular sample or irradiation time. These can be estimated using the displacement cross sections of a particular material and the neutron flux of the facility. If the displacement cross sections are not readily available, a suitably defined effective

³"Recommended Practice for Reporting Neutron Dosimetry Results on Graphite," *ASTM Standards* 45, E525 (1974).

Table 2. Effective graphite displacement cross sections

Neutron flux spectrum ^a	$E_L = 5.0 \times 10^{-4}$ eV		$E_L = 0.052$ MeV		$E_L = 0.183$ MeV	
	$\bar{\phi}(E_L)$	$\bar{\sigma}_D(E_L)$	$\bar{\phi}(E_L)$	$\bar{\sigma}_D(E_L)$	$\bar{\phi}(E_L)$	$\bar{\sigma}_D(E_L)$
	(n/cm ² sec $\times 10^{15}$)	(barns)	(n/cm ² sec $\times 10^{15}$)	(barns)	(n/cm ² sec $\times 10^{15}$)	(barns)
1	10^{-15}	169.9	0.258×10^{-15}	658.5	0.190×10^{-15}	894.6
2	10^{-15}	717.2	0.994×10^{-15}	721.6	0.963×10^{-15}	744.4
3	0.257	85.56	0.032	685.3	0.028	797.9
4	0.0649	63.15	0.0060	685.8	0.0052	781.3
5	1.0	786.3	0.421	679.5	0.354	809.1
6	1.0	278.5	0.408	683.1	0.346	804.8
7	6.1	166.4	1.48	685.4	1.26	806.0
8	3.0	138.8	0.624	666.8	0.495	840.5
9	5.9	200.0	1.72	686.8	1.47	803.9
10	3.1	614.6	2.91	655.8	2.34	812.6

^aSpectrum

Neutron flux spectrum descriptions

- 1 Normalized large HTGR spectrum (Don Matthews, GA)
- 2 Normalized ²³³U fission spectrum
- 3 Neutron flux 2.51 in. into ORR poolside
- 4 Neutron flux 5.65 in. into ORR poolside
- 5 Neutron flux at center of E-3 facility of ORR
- 6 Neutron flux at edge of E-3 facility of ORR
- 7 Neutron flux of HFIR target
- 8 Neutron flux of HFIR RB-3 facility
- 9 Neutron flux of HFIR PTP facility
- 10 Neutron flux for horizontal midplane of row Z of EBR-2

neutron damage fluence can be used. Damage fluences are widely used as a comparative basis.

Consider two irradiation facilities, A and B, each with a characteristic energy dependent neutron flux, $\phi_A(E)$ and $\phi_B(E)$. Then for a given material, effective displacement cross sections and fluxes are given by:

$$\bar{\sigma}_D^A(E_L) = \frac{\int_0^\infty \sigma_D(E) \phi_A(E) dE}{\int_{E_L}^\infty \phi_A(E) dE} = \frac{D_A}{\bar{\phi}_A(E_L)},$$

and

$$\bar{\sigma}_D^B(E_L) = \frac{\int_0^\infty \sigma_D(E) \phi_B(E) dE}{\int_{E_L}^\infty \phi_B(E) dE} = \frac{D_B}{\bar{\phi}_B(E_L)}.$$

If the number of displacements in A is equal to the number of displacements in B, then:

$$\bar{\sigma}_D^A(E_L) \bar{\phi}_A(E_L) t_A = \bar{\sigma}_D^B(E_L) \bar{\phi}_B(E_L) t_B = \text{total displacements},$$

where

t_A = irradiation time in facility A,

t_B = irradiation time in facility B,

$\bar{\phi}_A(E_L) t_A$ = effective damage fluence in facility A above E_L ,

$\bar{\phi}_B(E_L) t_B$ = effective damage fluence in facility B above E_L .

Note that equal damage fluence, $\bar{\phi}_A(E_L) t_A$ and $\bar{\phi}_B(E_L) t_B$, will produce equal displacements only under the special circumstance $\bar{\sigma}_D^A(E_L) = \bar{\sigma}_D^B(E_L)$. However, the effective cross sections are generally not equal so that equal damage fluences do not generally result in equal total displacements.

For many years, graphite displacement data from reactor facilities have been compared on the basis of neutron fluences above $E_L = 0.18$ MeV without regard for differences in effective displacement cross sections. The justification for initiating this practice resulted from the following observations. The high energy portion of the neutron energy spectra in

most reactor facilities is very similar and is also responsible for most displacements in graphite. Therefore, by choosing the right cutoff energy, E_L , the effective displacement cross sections for most reactor spectra would have nearly the same value, and intercomparisons could be based solely on fluence above E_L . The cutoff energy of 0.18 MeV was selected on this basis in some previous evaluation.

Damage Fluence Above 0.18 MeV

A recent evaluation has been made of the effective graphite displacement cross section, $\bar{\sigma}_D(E_L)$, at several cutoff energies, E_L , for a variety of reactor spectra of current interest. Figure 2 shows $\bar{\sigma}_D(E_L)$ versus E_L for these spectra. (These energy spectra are also referred to in Table 2 and are plotted in Figs. 3 through 12.) As can be seen, $\bar{\sigma}_D(E_L)$ has nearly the same value for all the neutron energy spectra when $E_L = 0.18$ MeV. Therefore, when $E_L = 0.18$ MeV is used as the cutoff energy, relative damage fluences will be nearly equivalent to relative displacement number. Note, however, that the $\bar{\sigma}_D(E_L)$ are even closer when $E_L = 0.052$ MeV. This suggests that the basis for comparing graphite displacement data from different facilities should be neutron fluences with $E_L = 0.052$ MeV rather than $E_L = 0.18$ MeV.

The observation that the damage fluence above 0.18 MeV is nearly proportional to the number of atoms displaced originally led to the practice of comparing graphite displacement data from different facilities solely on the basis of neutron fluence above 0.18 MeV. However, more detailed comparisons should incorporate all available information, and calculations of displacement rates and total displacements should be made. Displacement damage data from different irradiation facilities can be compared on the basis of these two characteristics.

Equivalent Fission Fluence, Φ_G

Other displacement damage characteristics have been defined for use in comparison of damage in graphite. The "equivalent fission fluence for damage in graphite" Φ_G is defined as follows:

Fig. 2. Effective graphite displacement cross section versus cut-off energy for various reactor spectra.

Fig. 3. HTGR spectrum (GA).

Fig. 4. ²³³U fission spectrum (ENDF-IV).

Fig. 5. Calculated neutron flux spectrum 2.51 in. into ORR poolside.

Fig. 6. Calculated neutron flux spectrum 5.65 in. into ORR poolside.

Fig. 7. Calculated neutron flux spectrum at center of E-3 facility of ORR.

Fig. 8. Calculated neutron flux spectrum at edge of E-3 facility of ORR.

Fig. 9. Calculated neutron flux spectrum in HFIR target.

Fig. 10. Calculated neutron flux spectrum in RB-3 facility of HFIR.

Fig. 11. Calculated neutron flux spectrum in HFIR PTP facility.

Fig. 12. Calculated neutron flux spectrum in row 2 HMP of EBR-II.

$$\Phi_G = \frac{\int_{t_1}^{t_2} \int_0^{\infty} \sigma_D(E) \phi(E,t) dE dt}{\int_0^{\infty} \sigma_D(E) \chi(E) dE / \int_0^{\infty} \chi(E) dE},$$

or

$$\Phi_G = \frac{\text{total displacements}}{\bar{\sigma}_x},$$

where

$t_2 - t_1$ = duration of the irradiation test,

$\bar{\sigma}_x$ = fission spectrum average cross section,

$\phi(E,t)$ = neutron flux in the irradiation test.

Physically, Φ_G is the fluence required in a fission spectrum to produce the number of displacements that occurred in a particular irradiation test. The "equivalent fission fluence" is widely used and is described in detail in Ref. 3.

Equivalent HTGR Fluence, Φ_{HTGR}

Another parameter, the "equivalent HTGR fluence for damage in graphite" is defined as follows:

$$\Phi(E_L)_{HTGR} = \frac{\int_0^{\infty} \int_{t_1}^{t_2} \sigma_D(E) \phi(E,t) dt dE}{\int_0^{\infty} \sigma_D(E) \phi(E)_{HTGR} dE / \int_{E_L}^{\infty} \phi(E)_{HTGR} dE},$$

$$\Phi(E_L)_{HTGR} = \frac{\text{total displacements}}{\bar{\sigma}(E_L)_{HTGR}},$$

where

$\bar{\sigma}_{HTGR}$ = effective displacement cross section for an HTGR spectrum above energy E_L ,

$\phi(E,t)$ = neutron flux in the irradiation test,

$\Phi(E_L)_{HTGR}$ = equivalent HTGR fluence for damage in graphite for energy above E_L .

Physically, $\Phi(E_L)_{\text{HTGR}}$ is the neutron fluence above energy E_L which a specimen must experience in a reference HTGR flux spectrum to produce the same number of atom displacements that occurred in a particular irradiation test. This convention is particularly useful for reporting graphite irradiation data from various test facilities in a form directly applicable to HTGRs.

Considerable graphite test data have previously been reported in terms of neutron fluences in the various test facilities, and intercomparisons of these data require translation of the reported fluences into a common parameters such as the equivalent HTGR fluence above some cutoff energy E^* . This translation can be accomplished by defining a conversion factor $f_R(E_L)$ as follows:

$$\Phi(E^*)_{\text{HTGR}} = \frac{\bar{\sigma}(E_L)_R}{\bar{\sigma}(E^*)_{\text{HTGR}}} \times \Phi(E_L)_R = f_R^*(E_L) \times \Phi(E_L)_R ,$$

where

R = subscript denoting a particular irradiation test,

$$f_R^*(E_L) = \bar{\sigma}(E_L)_R / \bar{\sigma}(E^*)_{\text{HTGR}} ,$$

E^* = specified cutoff energy for HTGR spectrum (not necessarily the same as E_L),

The other terms are as previously defined. Note that the conversion factor is a ratio of effective displacement cross sections and is, therefore, dependent on both the cutoff energy E_L and the neutron energy spectra used to obtain the effective cross sections. The neutron energy spectrum in a given irradiation test is dependent on both the irradiation facility and the test capsule composition, so that a unique conversion factor must be defined for each irradiation test. However, for practical purposes a conversion factor can be defined for similar capsules in a given facility. Some typical values of interest to the HTGR program are given in Table 3.

Equivalent DIDO Nickel Fluence (EDNF)

A convention commonly used in Europe for correlating irradiation damage in graphite is the "Equivalent DIDO Nickel Flux (EDNF)." This convention was developed because many of the early irradiations for studying

Table 3. Factors to convert damage fluences in test facilities to equivalent HTGR fluences^a above 0.183 MeV

Test facility ^b R	$f_R^*(E_L)$		
	$E_L = 5 \times 10^{-4}$ eV	$E_L = 0.052$ MeV	$E_L = 0.183$ MeV
1	0.190	0.736	1.000
2	0.802	0.807	0.832
3	0.096	0.766	0.892
4	0.071	0.767	0.873
5	0.879	0.760	0.904
6	0.311	0.764	0.900
7	0.186	0.766	0.901
8	0.155	0.745	0.940
9	0.224	0.768	0.899
10	0.687	0.733	0.908

$$^a \phi(E > 0.183 \text{ MeV})_{\text{HTGR}} = f_R^*(E_L) \times \phi(E_L)_R$$

^b Spectrum

Neutron flux spectrum descriptions

1	Normalized large HTGR spectrum (Don Matthews, GA)
2	Normalized ²³³ U fission spectrum
3	Neutron flux 2.51 in. into ORR poolside
4	Neutron flux 5.65 in. into ORR poolside
5	Neutron flux at center of E-3 facility of ORR
6	Neutron flux at edge of E-3 facility of ORR
7	Neutron flux of HFIR target.
8	Neutron flux of HFIR RB-3 facility
9	Neutron flux of HFIR PTP facility
10	Neutron flux for horizontal midplane of row Z of EBR-2

graphite damage were made in the DIDO reactor, and this reactor was selected as a convenient reference neutron source. The EDNF is defined as the nickel flux in DIDO which will produce the same graphite damage as the reactor under consideration; the Equivalent DIDO Nickel Dose (EDND) is the time integrated EDNF.

A nickel flux, ϕ_{Ni} , can be defined for a reactor with a neutron flux spectrum $\phi(E)$ by:

$$\phi_{Ni} = \int_0^{\infty} \sigma_{Ni}(E) \phi(E) dE / \hat{\sigma}_{Ni} = RR_{Ni} / \hat{\sigma}_{Ni},$$

where

ϕ_{Ni} = the nickel flux in the reactor,

$\sigma_{Ni}(E)$ = the differential cross section for the $^{58}Ni(n,p)$ reaction,

$\phi(E)$ = the neutron flux spectrum in the reactor,

$\hat{\sigma}_{Ni}$ = the fission spectrum averaged cross section for the $^{58}Ni(n,p)$ reaction,

RR_{Ni} = the atomic reaction rate for the $^{58}Ni(n,p)$ reaction.

The $^{58}Ni(n,p)$ reaction rate can be determined experimentally or can be calculated if the neutron flux spectrum is known. Several years ago, the neutron flux spectrum was determined for a specific position in a selected DIDO reactor configuration. This spectrum was then used to calculate a DIDO nickel flux ϕ_{Ni}^* using the preceding definition. The same DIDO spectrum was used to calculate an atom displacement rate for graphite, N_d^* , in the DIDO facility by:

$$N_d^* = \int_0^{\infty} \sigma_d(E) \phi^*(E) dE,$$

where

$\sigma_d(E)$ = the graphite displacement cross section,

$\phi^*(E)$ = the specified DIDO spectrum.

An effective graphite displacement cross section based on the DIDO nickel flux could then be defined:

$$\bar{\sigma}_d^* \equiv \frac{N_d^*}{\phi_{Ni}^*}.$$

Results from graphite irradiations in other facilities can be related to results from the DIDO irradiations. For example, if the graphite displacement rate, N_d^R , for some reactor is known, then the equivalent DIDO nickel flux for this reactor can be expressed as:

$$EDNF = \frac{N_d^R}{\bar{\sigma}_d^*}.$$

When the graphite displacement rate in the reactor is not known, the reactor spectrum can be assumed identical to that in DIDO. Then a nickel flux, ϕ_{Ni}^R , can be experimentally determined for the reactor and used to estimate the graphite displacement rate in the reactor:

$$N_d^R \approx \phi_{Ni}^R \bar{\sigma}_d^*.$$

However, this approach is limited by the assumed spectral similarity.

CONCLUSIONS

Several conventions for intercomparison of graphite irradiation data have been described. In each of these conventions there is an implied knowledge of the detailed neutron flux spectrum in the neutron energy range where graphite displacements occur. Unfortunately, the neutron spectra in most irradiation facilities are not well known and, regardless of the convention used, intercomparisons are limited by uncertainties in the neutron spectra.

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