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CALCULATED DAMAGE FUNCTIONS
FOR DETERMINING
IRRADIATION EFFECTIVENESS

September 1969

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CALCULATED DAMAGE FUNCTIONS
FOR DETERMINING
IRRADIATION EFFECTIVENESS

By

G. E. Russcher

Engineering Department
FFTF Division

September 1969

BATTELLE MEMORIAL INSTITUTE
PACIFIC NORTHWEST LABORATORIES
RICHLAND, WASHINGTON 99352

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ABSTRACT

This report provides data for a technique which a development engineer or a designer can use to estimate the effectiveness of two or more reactor spectra in producing irradiation damage. Using this technique permits the calculation of the fluence in a reactor environment under design that is equivalent to the fluence which produced a measured materials property change in an irradiation environment.

Included is a tabulated irradiation damage function that can be used to correlate irradiation spectra in terms of their relative effectiveness in producing damage. Two damage weighting functions have also been tabulated.

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CALCULATED DAMAGE FUNCTIONS
FOR DETERMINING IRRADIATION EFFECTIVENESS

G. E. Russcher

INTRODUCTION

Irradiation environments should be correlated on the basis of their effectiveness in producing radiation damage. Experimental irradiation data should not be directly applied to reactor design problems, because different neutron spectra can produce different kinds and quantities of damage. This report provides data for a technique which a development engineer or a designer can use to estimate the effectiveness of two or more reactor spectra in producing irradiation damage. Using this technique permits the calculation of the fluence in a reactor environment under design that is equivalent to the fluence which produced a measured materials property change in an irradiation environment.

Irradiation effectiveness is calculated with the use of irradiation damage weighting functions that are tabulated in this report. The tabulated weighting functions are presented for HOMSET and COMPRASH neutron energy group structures, which are currently used for Battelle-Northwest (BNW) and Westinghouse neutron shielding computations and for the Russian neutron energy group structure used for core physics computations. To illustrate the calculation of irradiation effectiveness of two spectra, example calculations for the EBR-II core Row 2 midplane and the vertical core FTR tube sheet spectra are included.

The calculated damage functions are for stainless steel and the calculated irradiation has no fluence limit since the effectiveness is based on fluences that produce the same damage. The damage functions relate irradiation effectiveness only in terms of differences in neutron spectra and other

parameters such as material, purity, and temperature must be held constant to obtain meaningful correlations.

A discussion of the physical basis for this correlation technique, and the development of the damage weighting functions are presented in the appendix. This report serves primarily to direct the application of the technique.

CONCLUSION

This report contains a tabulated irradiation damage function that can be used to correlate irradiation spectra in terms of their relative effectiveness in producing damage.

The weighting technique has been specifically designed to the engineering and design needs of Westinghouse and Battelle-Northwest where the COMPRASH, HOMSET, and Russian neutron group structures are used in reactor physics calculations.

Two damage weighting functions have been tabulated. The gross displacement function is probably the most conservative. The large vacancy cluster function, $N \geq 10$, is the most restrictive and perhaps underestimates damage since only the most stable form of clustered damage is calculated, however, it is currently believed to be the most responsive damage function to mechanical property radiation damage.

IRRADIATION DAMAGE FUNCTIONS

Irradiation damage weighting factors are presented in Tables 1, 2, and 3 for the HOMSET, COMPRASH, and Russian neutron group structures. Two weighting functions are given representing the production of gross lattice displacements and the production of clusters of 10 or more vacancies.

The damage weighting functions are intended to give a preliminary indication of the damaging effectiveness of neutron spectra for design purposes. This is accomplished by calculating the damage produced by two or more neutron spectra using the

damage function that is most conservative or best represents the experimental data of interest.

The gross displacement damage function is the more conservative since it includes all lattice displacements produced, even those that may subsequently anneal out. Probably only 1% of these displacements remain after irradiation at 900 °F.

TABLE 1. *Neutron Damage Function Weighting Factors for HOMSET Group Structure*

HOMSET Group Number	Neutron Lower Limit Energy, eV	Weighting Factors	
		Gross Displacements (F_{GD})	Clustered Vacancies (F_{CV10})
			$N \geq 10$
0	1.0 $\times 10^7$	100.0	4.0
1	6.065 $\times 10^6$	109.8	4.2881
2	3.679	113.5	4.3885
3	2.231	119.3	4.619
4	1.353	101.8	4.180
5	8.209 $\times 10^5$	72.14	2.936
6	3.877	51.61	2.222
7	1.832	24.43	1.076
8	6.738 $\times 10^4$	15.25	0.6884
9	2.479	10.70	0.1393
10	1.930	5.603	0
11	9.119 $\times 10^3$	3.329	0
12	3.355	0.9642	0
13	1.234	0.689	0
14	4.54 $\times 10^2$	0.09558	0
15	2.754	0.02219	0
16	2.145	0.007966	0
17	1.013	0.01323	0
18	6.144 $\times 10^1$	0.01296	0
19	2.902	0.01751	0
20	1.371	0.02540	0
21	1.068	0.03335	0
22	3.928	0.04278	0
23	1.445	0.06977	0
24	0.9764	0.1015	0
25	0.6826	0.1198	0
26	0.4140	0.1466	0
27	0.2775	0.1829	0
28	0.1860	0.2282	0
29	0.1247	0.2826	0
30	0.07595	0.3448	0
31	0	0.7631	0

TABLE 2. *Neutron Damage Function Weighting
Factors for COMPRASH Group Structure*

COMPRASH Group Number	Neutron Lower Limit Energy, eV	Weighting Factors	
		Gross Displacements (F_{GD})	Clustered Vacancies (F_{CV10}) $N \geq 10$
0	1.0×10^7	100.0	3.8
1	8.5×10^6	100.1	3.931
2	7.5	111.3	4.345
3	6.5	114.1	4.445
4	5.5	114.7	4.452
5	4.5	117.1	4.519
6	3.5	120.4	4.631
7	2.5	121.5	4.689
8	1.5	104.5	4.291
9	8.0×10^5	74.87	3.054
10	4.0	51.66	2.225
11	1.0	21.72	0.9509
12	5.0×10^4	11.98	0.4498
13	1.5	7.170	0
14	5.0×10^3	2.604	0
15	1.5	1.779	0
16	5.0×10^2	0.5775	0
17	1.5	0.01607	0
18	5.0×10	0.01325	0
19	1.5	0.02103	0
20	5.0	0.03723	0
21	1.5	0.06406	0
22	0.55	0.1089	0
23	0.14	0.1920	0
24	0	0.5635	0

TABLE 3. *Neutron Damage Function Weighting Factors for Russian(a) Group Structure*

Russian Group Number	Neutron Lower Limit Energy, eV	Weighting Factors	
		Gross Displacements (F_{GD})	Clustered Vacancies (F_{CV10}) $N \geq 10$
0	10.5×10^6	100.0	4.000
1	6.5	108.87	4.255
2	4.0	116.81	4.510
3	2.5	121.27	4.678
4	1.4	103.28	4.241
5	8.0×10^5	72.29	2.947
6	4.0	51.24	2.206
7	2.0	26.69	1.1715
8	1.0	17.268	0.7702
9	4.65×10^4	11.841	0.4165
10	2.15	8.110	0.03714
11	1.0	3.728	0
12	4.65×10^3	1.6066	0
13	2.15	1.6740	0
14	1.0	0.6346	0
15	4.65×10^2	0.07838	0
16	2.15	0.01385	0
17	1.0	0.01322	0
18	4.65×10^1	0.01440	0
19	2.15	0.02017	0
20	1.0	0.03105	0
21	4.65	0.04230	0
22	2.15	0.06206	0
23	1.0	0.09287	0
24	0.465	0.1308	0
25	0.215	0.1872	0
26	0	0.5313	0

(a) Group Constants for Nuclear Reactor Calculations,
I. I. Bondarenko, Ed., translated from the Russian
by Consultants Bureau, New York, 1964.

The vacancy cluster damage function for $N \geq 10$ is less conservative but probably more representative of damage produced by irradiation at temperatures up to 900 °F. Computer calculations have shown the 10 vacancy clusters to be stable at simulated high temperatures, therefore, clusters of 10 or more vacancies may better represent mechanical property changes such as radiation induced strengthening.^(1,2) A neutron of at least 25 keV is effectively required to produce a cluster of 10 or more vacancies.

Comparative irradiation effectiveness is the ratio of fluences that produce the same damage in the two irradiation environments. Experimental data should be selected that are for the exact material, composition, purity, metallurgical history, and materials property measurements as are needed in the design application. Each represents a variable that influences the formation of radiation damage. The neutron spectrum is an influential variable of an environment, and it is the basis of the irradiation effectiveness. Since the damage weighting functions relate irradiation effectiveness only in terms of neutron spectral differences, the other variables must be maintained constant to ensure meaningful data correlation.

Computer simulated damage production has shown that damage production rates change with increasing irradiation fluence. The changes are determined by the accumulated concentration of irradiation damage. Since the effectiveness is based on fluences that produce the same damage, changes in damage production rates apply equally to the irradiation environments. As a result, this calculated irradiation effectiveness has no fluence restrictions.

APPLICATION OF THE DAMAGE FUNCTION WEIGHTING FACTORS

The comparative irradiation effectiveness of two or more neutron spectra is calculated by weighting their spectra with

a damage function. Each neutron spectrum should be described as normalized, integrated flux or fluence in HOMSET, COMPRASH, or Russian group structure; then a damage function should be selected. The neutron fraction in each group or tabular distribution should be multiplied by the damage weighting factor for that group. These weighted products should then be summed over the entire group structure. That sum is the calculated damage per unit fluence or flux in a unit volume of stainless steel.

A similar computation should be done for the other neutron spectra to be correlated. The weighted sum is the calculated damage per unit fluence or flux. The ratio of the calculated weighted sums represents the ratio of fluences that produces the same damage. Example calculations compare the gross displacement production at the EBR-II midplane Row 2 with gross displacement production at the FTR tube sheet location.

The spectra of the EBR-II and FTR-TS have been tabulated in Tables 4 and 5, and the damage weighting factors are applied to them, illustrating how the calculation is performed. The result is

$$\frac{D_{\text{EBR-II}}/\phi_{\text{EBR-II}}}{D_{\text{FTR-TS}}/\phi_{\text{FTR-TS}}} = \left[\frac{\phi_{\text{FTR-TS}}}{\phi_{\text{EBR-II}}} \right] = \frac{52.33^{(a)}}{3.15} = 16.59$$

D=const.

Thus, an irradiation to 17×10^{20} total n/cm² in FTR tube sheet would produce the same damage as an irradiation to 10^{20} total n/cm² in the EBR-II core.

(a) This reference spectrum value is 2.2 using the clustered vacancy function.

TABLE 4. EBR-II Damage Calculation (Row 2 Midplane)

HOMSET Group Number	Group Lower Limit Energy (E _L)	Neutron Spectrum		Weighting Factor Gross Displacements (F _{GD})	Damage (D), TD × F _{GD}
		Integral Distribution (ID)	Tabular Distribution (TD)		
0	10 MeV	1.00	0.	100.0	0.
1	6.065	0.993	0.007	109.8	0.7686
2	3.679	0.96	0.033	113.5	3.746
3	2.231	0.89	0.070	119.3	8.348
4	1.353	0.79	0.10	101.8	10.184
5	0.8209	0.67	0.12	72.14	8.657
6	0.3877	0.43	0.24	51.61	12.386
7	0.1832	0.20	0.23	24.43	5.619
8	0.06738	0.07	0.13	15.25	1.983
9	0.02479	0.015	0.055	10.70	0.5883
10	0.01930	0.010	0.005	5.603	0.0280
11	9.119 keV	0.002	0.008	3.329	0.0266
12	3.355	0.0003	0.0017	0.9642	0.0016
13	1.234	0.	0.0003	0.6890	0.0002
14	0.454	0.	0.	0.09558	0.
15	0.2754	0.	0.	0.02219	0.
			1.000		52.335

TABLE 5. FTR Tube Sheet Damage Calculation

HOMSET Group Number	Group Lower Limit Energy (E_L)	Neutron Spectrum		Weighting Factor Gross Displacements (F_{GD})	Damage (D), $TD \times F_{GD}$
		Integral Distribution (ID)	Tabular Distribution (TD)		
0	10 MeV	1.0000	0.	100.0	0.
1	6.065	0.99999	0.00001	109.8	0.00110
2	3.679	0.999974	0.000016	113.5	0.00182
3	2.231	0.99990	0.000074	119.3	0.00883
4	1.353	0.99956	0.0034	101.8	0.03463
5	0.8209	0.99835	0.00121	72.14	0.08729
6	0.3877	0.9912	0.00725	51.61	0.3742
7	0.1832	0.9695	0.0217	24.43	0.5302
8	0.06738	0.906	0.0635	15.25	0.9684
9	0.02479	0.838	0.068	10.70	0.7273
10	0.01930	0.818	0.020	5.603	0.1121
11	9.119 keV	0.760	0.058	3.329	0.1931
12	3.355	0.705	0.055	0.9642	0.0530
13	1.234	0.655	0.050	0.689	0.03445
14	0.454	0.555	0.10	0.09558	0.00956
15	0.2754	0.505	0.05	0.02219	0.00111
16	0.2145	0.480	0.025	0.00796	0.00020
17	0.1013	0.400	0.08	0.01323	0.00106
18	61.44 eV	0.345	0.055	0.01296	0.00071
19	29.02	0.260	0.085	0.01751	0.00149
20	13.71	0.185	0.075	0.02540	0.00191
21	10.68	0.163	0.022	0.03335	0.00073
22	3.93	0.092	0.071	0.04278	0.00304
23	1.445	0.042	0.050	0.06977	0.00349
24	0.876	0.	0.0419	0.1015	0.00430
25	0.	0.	0.	0.1198	0.
			1.0000		3.15390

The neutron spectra of the example problems were not available in either HOMSET or COMPRASH neutron group structures during the preparation of this report, so the spectra were first converted to integral distributions. The smooth integral function was then converted to a HOMSET tabular distribution by subtracting the integral distribution for the group lower energy from the integral distribution for the upper energy. Other neutron spectra can be converted to tabular structure this way, or they can be inexpensively converted by a brief computer program that is available.

APPENDIX

CALCULATION METHOD AND DEVELOPMENT
OF DAMAGE WEIGHTING FACTORS

APPENDIX

CALCULATION METHOD

The physical basis for the development of the damage correlation technique is briefly described. Radiation interactions, interatomic collisions, crystal lattice behavior, and damage center production are considered. These physical processes and their environmental conditions are discussed as influences on calculated irradiation damage.

Irradiation damage is calculated with the help of several computer programs designed to simulate the production of irradiation damage and the results are tabulated as damage functions. The process is illustrated in Figure 1. The first stage of the computations operates on individual neutron groups. For example, using unit fluence in the fifth group of the HOMSET structure, the calculations yield the probable neutron interactions that can produce primary knocked-on atoms, PKAs. These PKA produced by the H-5 neutrons have a characteristic energy distribution, schematically illustrated in Figure 1. The second stage of the computations is the calculation of the kinds of damage that the distribution of PKAs can produce. Two different kinds of damage, gross displacement production, and clustered vacancy production are calculated and tabulated to give the entry for the H-5 group in the weighting factor table (Tables 1 and 2). These steps are repeated with each energy group to complete the tables. This series of computations has been executed for the HOMSET, COMPRASH, and Russian neutron energy groups.

DEVELOPMENT OF DAMAGE WEIGHTING FACTORS

Several computer programs are used to calculate the weighting factors that represent irradiation damage done by a group of neutrons with a specific energy. As the neutrons impinge on a specimen, their interaction probability is

FIGURE 1. Calculation Method Schema

determined by the cross sections for the elements making up the specimen. The interactions considered that can cause lattice structure damage are neutron scattering collisions and $(n\gamma)$ recoils. These atoms set in motion by either interaction are called primary knocked-on atoms (PKAs). Both the production probability and the PKA energy are calculated. These PKA subsequently traverse the crystal lattice specimen, colliding with other atoms, displacing many from their lattice sites, and often forming cascades of displacements. The numbers and configurations of the displacements are calculated, and tabulated in two categories: (1) the gross number of lattice displacements, and (2) the number of clustered vacancies that are produced in these displacement cascades. The number of gross displacements includes all those displacements produced (as if at 0 °K) except for Frenkel pairs which spontaneously recombine within an Erginsoy volume of 32 lattice sites. The number of clustered vacancies tabulated are those produced in clusters of at least ten; clusters that are stable to temperatures as high as 900 °F.

COMPUTATION DETAILS

The first stage in the computation of irradiation damage produced by a group of neutrons uses the SPECTRA computer program. Each neutron energy group is represented in the SPECTRA computation by a neutron with the mean lethargy or logarithmic energy of that neutron group. For the j^{th} group, for example, that mean lethargy is

$$\bar{\mu}_j = \frac{\ln(E_j) - \ln(E_{j-1})}{2} \quad (1)$$

The energy transferred to atoms of the specimen are calculated by SPECTRA, using anisotropic scattering cross sections for the major elements of stainless steel (Fe, Ni, and Cr), the element atomic densities and their atomic masses. The energy

transferred to a PKA is calculated in center-of-mass (C.M.) coordinates, hence, the C.M. scattering cross sections are used.⁽³⁾ They are assembled in a data matrix of 21 scattering angles and 100 neutron energy values.

$$E_T = E[1 - 1/2 \{(1 - \beta) + (1 - \beta) \cos \phi\}] - E_D \quad (2)$$

where $\beta = \frac{(A - 1)^2}{(A + 1)}$ and $\cos \phi =$ C.M. scattering angle cosine. Ten thousand calculations are made for each neutron energy group to provide a probable PKA energy distribution for that group.

Another computer program, SAND-II, is used to compute the nuclear activation, $\text{Fe}(n, \gamma)$, which leads to iron recoil damage.

$$A_{\text{Fe}^{59}} = \frac{N_{\text{Fe}} \int_{E_j}^{E_{j-1}} \phi(E) \sigma(E) dE}{\int_{E_j}^{E_{j-1}} \phi(E) dE} \quad (3)$$

Neutron capture by iron is computed for each neutron group using the atomic density of iron in stainless steel (N_{Fe}) and the energy dependent activation cross section data. The number of captures per unit volume of the specimen and unit fluence represent the number of recoil PKAs generated. As the γ spectrum is emitted with a predominate energy of 7.6 MeV, the iron atom recoils with a calculated average energy of 390 eV.⁽⁴⁾

These recoils are added to the 380-400 eV PKA group from the SPECTRA calculation. This total PKA distribution then represents the conclusion of the first calculation stage.

The next stage is subdivided into two parallel paths. There are several ways in which PKAs can disrupt a perfect crystal lattice. One is based on a gross displacement model developed by J. R. Beeler, Jr.⁽⁵⁾ and derived in part from the

Thompson and Wright model. The model, graphically shown in Figure 2, gives the number of gross displacements produced per unit volume of the specimen by a unit fluence. The portion of the relation below 20 keV was developed by computer simulation with the CASCADE-CLUSTER programs.⁽⁵⁾ The higher energy portion of the relation was developed with the method of Thompson and Wright,⁽⁶⁾ incorporating a mixture of elastic and inelastic atomic scattering. The composite damage model is used to calculate the gross displacements produced by the PKA spectrum from each neutron group.

Another way of computing the damage caused by the PKA spectrum is based on a clustered vacancy model, also shown in Figure 2.

The cluster size distribution as a function of PKA energy was also developed with a study using the CASCADE-CLUSTER computer programs.⁽⁵⁾ Probable cluster size distribution was calculated for PKA energies ranging from 0.5 to 20 keV. These size distributions have been used to calculate the number of vacancies that are found in large ($N \geq 10$) stable clusters from the various PKA spectra.

These damage functions represent different quantities and types of damage that PKAs can produce as they traverse the specimen. The damage produced by the PKA spectrum from each neutron group yields the weighting factors for the group. They are entered as the damage function in Tables 1, 2, and 3. The damage functions are graphically displayed in Figure 3 as a function of neutron group mean lethargy.

FIGURE 2. Damage Produced by PKAs

FIGURE 3. Neutron Damage Functions

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