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RECENT DEVELOPMENTS IN NEUTRON DOSIMETRY AND RADIATION DAMAGE CALCULATIONS  
FOR FUSION-MATERIALS STUDIES

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**MASTER**

# RECENT DEVELOPMENTS IN NEUTRON DOSIMETRY AND RADIATION-DAMAGE CALCULATIONS FOR FUSION-MATERIALS STUDIES

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This paper is intended as an overview of activities designed to characterize neutron irradiation facilities in terms of neutron flux and energy spectrum and to use these data to calculate atomic displacements, gas production, and transmutation during fusion materials irradiations. A new computerized data file, called DOSFILE, has recently been developed to record dosimetry and damage data from a wide variety of materials test facilities. At present data are included from 20 different irradiations at fast and mixed-spectrum reactors, T(d,n) 14 MeV neutron sources, Be(d,n) broad-spectrum sources, and spallation neutron sources. Each file entry includes activation data, adjusted neutron flux and spectral data, and calculated atomic displacements and gas production. Such data will be used by materials experimenters to determine the exposure of their samples during specific irradiations. This data base will play an important role in correlating property changes between different facilities and, eventually, in predicting materials performance in fusion reactors. All known uncertainties and covariances are listed for each data record and explicit references are given to nuclear decay data and cross sections. Consequently, the data can easily be reviewed or readjusted in the future according to changes in nuclear data and new exposure parameters can be calculated if theoretical models are developed which go beyond displacements and transmutation.

The computer code package SPECTER has also been recently revised and updated to permit rapid calculation of displacements, gas production, and total dose for any given neutron spectrum. Recent improvements include new calculations with ENDF/B-V neutron cross sections, inclusion of (n, $\gamma$ ) and  $\beta$ -decay processes, inclusion of kerma cross sections for total dose, and the ENDF/B-V gas-production file. Users need only provide a neutron spectrum, with uncertainties if known, and the code will calculate spectral-averaged values of the above quantities as well as recoil atom distributions. Both the DOSFILE and SPECTER computer codes are readily accessible to the fusion community via the National Magnetic Fusion Energy Computer at Lawrence Livermore Laboratory.

## 1. INTRODUCTION

Fusion material studies are being conducted in a wide variety of neutron irradiation facilities, including fission reactors and particle accelerators. Since none of these sources duplicate the neutron flux or energy spectrum expected in a fusion reactor, we must be able to characterize each facility in terms of neutron exposure parameters and then use these data to calculate more fundamental damage parameters such as atomic displacements and gas production. Hopefully, materials property changes can then be correlated between these

*ESB*

different neutron sources and extrapolated to fusion reactor conditions. Consequently, an effort is now underway to characterize all fusion materials irradiation facilities in terms of these neutron and damage parameters.<sup>1</sup>

Two computer files have been developed to make the results of these source characterization efforts readily available to the fusion community. DOSFILE is a comprehensive file of measured and calculated exposure parameters for specific experiments at most fusion materials irradiation facilities, including fission reactors and accelerator-based neutron sources. The SPECTER computer code is available for calculating damage parameters. Users need only specify a neutron flux spectrum. The program will then provide spectral-averaged atomic displacements, gas production, total dose, and recoil atom distributions for 38 different elements spanning the periodic table. Both codes are available to users of the National Magnetic Fusion Energy Computer Center at Lawrence Livermore National Laboratory or directly from the author.

## 2. DOSFILE

The multiple activation technique is used to characterize neutron irradiation experiments.<sup>1</sup> In this method, activation products are measured by Ge(Li) gamma spectrometry from a variety of neutron reactions, each having a different energy response function. These measured activities are then used to adjust the neutron flux spectrum using the generalized least-squares computer code STAY'SL. The adjusted neutron spectrum is then used to calculate damage parameters using the computer code SPECTER, described later in this report.

The computer code DOSFILE has been developed to record and document the results of dosimetry measurements and damage calculations for fusion materials irradiations. On one level the code simply lists the activation measurements, adjusted flux spectrum, and computed damage parameters, each value having variance-covariances. However, the file also provides sufficient documentation and references sufficiently such that the data may be reanalyzed in the future if desired due to new nuclear data or damage models.

In order to simplify usage of the file, all sections are written in plain-English or with fairly obvious key words. The user need only specify which irradiations (Table I) and which topics (Table II) he is interested in. The program will then list the desired information. Each irradiation contains an identification (IDN) section which describes the irradiation history, specimen geometry, flux gradients (usually described by equations), and contains references to data files and publications. Uncertainties are provided for all input and output data. The output flux spectrum is listed with a complete covariance matrix since these data are required in order to determine uncertainties in calculated damage parameters and may be needed in future correlations with materials properties. If the user wishes to list the entire contents of one file or a particular topic for all files then the ALL key-word can be specified. Each irradiation file contains about 850 lines of data in a card-image format. A brief sample output is shown in Fig. 1.

At present, DOSFILE contains data on 20 separate irradiations, as listed in Table I. The file will be continually upgraded as new irradiation experiments

are completed. Also, some of our older experiments will be re-evaluated and added to the file.

### 3. SPECTER

The SPECTER computer code package contains extensive library data files of damage parameter cross sections in a 100 point energy grid. Users need only supply a neutron spectrum, with uncertainties if available. The code will then collapse the library cross sections to the user's energy grid and then proceed to average all quantities, keeping track of all uncertainties in the specified covariance matrix. Displacement damage cross sections were calculated for 38 elements using the computer code DISCS.<sup>3</sup> All neutron reaction cross sections were taken from ENDF/B-V.<sup>4</sup> The DISCS code calculates displacement damage and recoil atom energy distributions for elastic and inelastic scattering, (n,2n), (n,p), and (n, $\alpha$ ) reactions. Higher order reactions are lumped with one of these general categories. We have recently added a new treatment of the (n, $\gamma$ ) capture reaction and subsequent beta decay.<sup>5,6</sup>

Gas production cross sections are averaged from the ENDF/B-V Gas Production File 533.<sup>4</sup> Since this file only covers a limited number of elements, hydrogen and helium values are also listed from the general ENDF/B-V data files for all elements in our file. Total dose values (Kerma) are also provided using the MACKLIB<sup>7</sup> program.

The PKA recoil atom distributions require the largest amount of computer storage space. Each reaction is stored on a 100 point recoil energy grid at each of the 100 neutron energies thus making a total of 80,000 PKA values for each element. Users have the option of suppressing PKA calculations to speed up running time and reduce the printed output. Sample output are shown in Figs. 2-3. As can be seen, spectral-averaged data includes displacement damage cross sections, damage-energy cross sections, nuclear reaction cross sections, and gas production cross sections each with its associated uncertainty. The code also lists spectral averaged total dose (Kerma) and detailed PKA distributions for each reaction and element.

At present, only six elements have been extended to 50 MeV for use at Li or Be(d,n) and spallation neutron sources. Future work will focus on extending more data files to higher energies and on including more elements in our data files.

### REFERENCES

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Table I

## Irradiation Data Contained in DOSFILE

Irradiation*	Key Word
HFIR-CTR31	HFR31
HFIR-CTR32	HFR32
HFIR-CTR34	HFR34
HFIR-CTR35	HFR35
HFIR-T2	HFRT2
HFIR-RB1	HFRB1
ORR-MFE1	ORMF1
ORR-MFE2	ORMF2
ORR-MFE4A-1	OR4A1
ORR-MFE4A-2	OR4A2
ORR-Spectral Run	ORRLP
ORR-TBC07	ORRT7
ORR-TRIO-1	TRIO1
Omega West-Spectral Run	OMWSP
Omega West-HEDL-1	OMWH1
IPNS-9-VT2-REF	IPN9C
EERII-X287	EB287
CP5-Fission Converter	CP5FC
HFBR-VT15-2	HFBR2
HFBR-VT15-3	HFBR3

\*HFIR: High Flux Isotope Reactor (ORNL)  
 ORR: Oak Ridge Research Reactor (ORNL)  
 Omega West Reactor (LANL)  
 IPNS: Intense Pulsed Neutron Source (ANL-E)  
 EBR II: Experimental Breeder Reactor II (ANL-W)  
 CP5: Chicago Pile 5 (ANL)  
 HFBR: High Flux Beam Reactor (BNL)

Table II

## Data Key Words for DOSFILE

Key Word	Description
IDN	Identification, irradiation history, gradients, references
ACT	Activities with uncertainties, covers, and self-shielding
FLI	Input flux data
FUN	Input flux uncertainties
FLO	Output flux data
FCV	Output flux covariance matrix
FSM	Flux, fluence summary
DAM	Damage parameters (DPA, He)

## Figures

- Figure 1. Sample output from the DOSFILE program for the CTR32 irradiation in HFIR. The activities are quoted in units of product atom per target atom per second. Fluxes are in neutrons/cm<sup>2</sup>-s-MeV, averaged over each energy group (10<sup>-10</sup> -20 MeV).
- Figure 2. Spectral-averaged damage cross sections calculated using SPECTER for the CTR32 irradiation in HFIR. Displacement, damage-energy, and nuclear reaction cross sections are averaged for each reaction type. Uncertainties are derived from the flux covariance matrix.
- Figure 3. Spectral-averaged gas production cross sections calculated using SPECTER for the CTR32 irradiation in HFIR. The total fluence was  $4.78 \times 10^{22}$  n/cm<sup>2</sup>. Burnup corrections are required for <sup>6</sup>Li and <sup>10</sup>B.





HFIR CTR 32 MIDPLANE 100 MW

TITANIUM 1322

SPECTRAL AVG. DISP SIGMAS, EDL = 0.40000E-04 MEV TOTAL FLUENCE = 4.78373E+22 +/- 3.70 %

DPA = 1.0464E+01 HELIUM(APPM) = 5.3709E+00 HYDROGEN(APPM) = 2.4627E+01

ELASTIC	INELST	(N,2N)	(N,2N)P	(N,2N)SUM	CH1	CH2	SUM	
1.5176E+02	5.8294E+01	1.6675E-02	5.1851E-02	6.8550E-02	3.5695E-01	4.3025E-02	2.1053E+02	BARNS
1.5176E+01	5.8294E+00	1.6675E-03	5.1851E-03	6.8550E-03	3.5695E-02	4.3025E-03	2.1053E+01	KEV-BARNS
+/- 7.04%	+/- 5.75%	+/- 12.01%	+/- 12.12%	+/- 12.01%	+/- 5.19%	+/- 8.75%	+/- 6.39%	
6.0330E+00	1.1528E-01	1.1761E-05	3.5086E-05		5.1481E-04	1.1227E-04	6.1489E+00	NUCLEAR - BARNS
+/- 5.97%	+/- 7.00%	+/- 12.03%	+/- 12.14%		+/- 4.50%	+/- 4.46%	+/- 5.86%	

CAPTURE GAMMA DAMAGE = 8.2036E-01 KEV-B +/- 4.09% CS = 2.0225E+00 BARNS, TGAM = 400.0 EV

TOTAL DPA CROSS-SECTION = 2.1873E+01 KEV-B; OR 2.1873E+02 BARNS

IRON - 1326

SPECTRAL AVG. DISP SIGMAS, EDL = 0.40000E-04 MEV TOTAL FLUENCE = 4.78373E+22 +/- 3.70 %

DPA = 9.1455E+00 HELIUM(APPM) = 3.1944E+00 HYDROGEN(APPM) = 5.0028E+01

ELASTIC	INELST	(N,2N)	(N,2N)P	(N,2N)SUM	CH1	CH2	SUM	
1.2978E+02	5.7071E+01	1.8712E-02	5.7735E-02	7.6442E-02	6.6229E-01	8.9148E-02	1.8768E+02	BARNS
1.2978E+01	5.7071E+00	1.8712E-03	5.7735E-03	7.6442E-03	6.6229E-02	8.9148E-03	1.8768E+01	KEV-BARNS
+/- 6.99%	+/- 5.64%	+/- 12.08%	+/- 12.15%	+/- 12.00%	+/- 5.91%	+/- 9.66%	+/- 6.23%	
8.6295E+00	1.2214E-01	1.3282E-05	4.0015E-05		1.0458E-03	6.6776E-05	8.7528E+00	NUCLEAR - BARNS
+/- 3.68%	+/- 7.08%	+/- 12.09%	+/- 12.17%		+/- 4.61%	+/- 6.99%	+/- 3.63%	

CAPTURE GAMMA DAMAGE = 3.5033E-01 KEV-B +/- 4.04% CS = 8.5700E-01 BARNS, TGAM = 395.0 EV

TOTAL DPA CROSS-SECTION = 1.9118E+01 KEV-B; OR 1.9118E+02 BARNS

NICKEL - 1328

SPECTRAL AVG. DISP SIGMAS, EDL = 0.40000E-04 MEV TOTAL FLUENCE = 4.78373E+22 +/- 3.70 %

DPA = 9.8417E+00 HELIUM(APPM) = 4.3938E+01 HYDROGEN(APPM) = 6.1990E+02

ELASTIC	INELST	(N,2N)	(N,2N)P	(N,2N)SUM	CH1	CH2	SUM	
1.5077E+02	3.8844E+01	2.7965E-02	9.3597E-01	9.6394E-01	6.0388E+00	1.4800E+00	1.9809E+02	BARNS
1.5077E+01	3.8844E+00	2.7965E-03	9.3597E-02	9.6394E-02	6.0388E-01	1.4800E-01	1.9809E+01	KEV-BARNS
+/- 7.14%	+/- 5.58%	+/- 11.22%	+/- 9.68%	+/- 9.59%	+/- 6.25%	+/- 7.45%	+/- 6.14%	
1.4087E+01	8.3333E-02	1.9938E-05	8.1458E-04		1.2959E-02	9.1850E-04	1.4186E+01	NUCLEAR - BARNS
+/- 3.81%	+/- 6.65%	+/- 11.14%	+/- 9.66%		+/- 5.03%	+/- 5.53%	+/- 3.78%	

CAPTURE GAMMA DAMAGE = 7.6399E-01 KEV-B +/- 4.05% CS = 1.5244E+00 BARNS, TGAM = 491.0 EV

TOTAL DPA CROSS-SECTION = 2.0573E+01 KEV-B; OR 2.0573E+02 BARNS

HFIR CTR 32 MIDPLANE 100 MW  
SPECTRAL AVERAGED GAS PRODUCTION (ENDF 533)

	SIGMA (MB)	GAS (APPM)
LI6(N, HYDROGEN)	9.7882E-01	4.6824E+01
LI6(N, DEUTERIUM)	2.3394E+01	1.1191E+03
LI6(N, TRITIUM)	3.1126E+05	1.4890E+07
LI6(N, HELIUM)	3.1128E+05	1.4891E+07
LI7(N, DEUTERIUM)	3.4531E-03	1.6519E-01
LI7(N, TRITIUM)	4.5686E+00	2.1855E+02
LI7(N, HELIUM)	2.8447E+01	1.3608E+03
BE9(N, HYDROGEN)	4.6710E-06	2.2345E-04
BE9(N, DEUTERIUM)	5.0308E-06	2.4066E-04
BE9(N, TRITIUM)	6.1720E-04	2.9525E-02
BE9(N, HELIUM)	4.8723E+01	2.3308E+03
B10(N, HYDROGEN)	1.7095E+00	8.1780E+01
B10(N, DEUTERIUM)	2.7667E-01	1.3235E+01
B10(N, HELIUM)	1.2753E+06	6.1009E+07
B11(N, HYDROGEN)	4.7018E-05	2.2492E-03
B11(N, TRITIUM)	4.5617E-04	2.1822E-02
B11(N, X)HELIUM	9.8452E-03	4.7097E-01
C12(N, HYDROGEN)	3.5266E-05	1.6870E-03
C12(N, HELIUM)	4.5151E-01	2.1599E+01
N14(N, HYDROGEN)	6.1271E+02	2.9310E+04
N14(N, HELIUM)	1.5503E+01	7.4162E+02
F19(N, HYDROGEN)	2.2115E-01	1.0579E+01
F19(N, HELIUM)	4.6436E+00	2.2214E+02
AL27(N, HYDROGEN)	8.0259E-01	3.8394E+01
AL27(N, HELIUM)	1.7148E-01	8.2029E+00
SI28(N, HYDROGEN)	1.1873E+00	5.6796E+01
SI28(N, HELIUM)	5.7668E-01	2.7587E+01
TI(N, HYDROGEN)	5.1671E-01	2.4718E+01
TI(N, HELIUM)	1.1246E-01	5.3798E+00
V(N, HYDROGEN)	9.8645E-02	4.7189E+00
V(N, HELIUM)	5.7802E-03	2.7651E-01
CR(N, HYDROGEN)	7.9783E-01	3.8166E+01
CR(N, DEUTERIUM)	1.8507E-05	8.8531E-04
CR(N, TRITIUM)	2.8279E-05	1.3528E-03
CR(N, HELIUM3)	9.0368E-07	4.3230E-05
CR(N, HELIUM4)	3.9193E-02	1.8749E+00
MN55(N, HYDROGEN)	1.4163E-01	6.7752E+00
MN55(N, HELIUM)	3.4704E-02	1.6602E+00
FE(N, HYDROGEN)	1.0707E+00	5.1222E+01
FE(N, HELIUM)	6.9787E-02	3.3384E+00
CO59(N, HYDROGEN)	2.8617E-01	1.3690E+01
CO59(N, HELIUM)	3.4375E-02	1.6444E+00
NI(N, HYDROGEN)	1.2970E+01	6.2044E+02
NI(N, DEUTERIUM)	2.5831E-03	1.2357E-01
NI(N, HELIUM)	9.1864E-01	4.3945E+01
CU(N, HYDROGEN)	2.2322E+00	1.0678E+02
CU(N, HELIUM)	6.2302E-02	2.9804E+00