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RADIATION DAMAGE AT THE ROTATING TARGET NEUTRON SOURCE (RTNS-I) FACILITY AT LAWRENCE LIVERMORE LABORATORY

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MASTER

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RADIATION DAMAGE AT THE ROTATING TARGET NEUTRON SOURCE (RTNS-I) FACILITY AT LAWRENCE LIVERMORE LABORATORY

Abstract

Some of the basic computational features of a computer program used for modeling radiation damage at LLL's Rotating Target Neutron Source (RTNS-I) are presented. Input items required are material cross-section and angular distribution data, such as used for LLL neutron transport calculations, along with one particular neutron spectrum of interest. The nuclear reactions considered are elastic,

neutron-emitting, and charged-particle-emitting. Classical and relativistic mechanics are used as required to calculate the resulting primary-recoil energy spectra and damage energy spectra. Calculative results are presented for the RTNS-I neutron spectra on aluminum, titanium, vanadium, iron, nickel, copper, zirconium, niobium, molybdenum, silver, tin, tantalum, tungsten, gold, and lead.

Introduction

In the early days of reactor technology and radiation damage, neutron fluence was used as a measure of radiation exposure. Radiation environments will continue to increase in complexity, especially as fusion reactors become a reality. The understanding of the fundamental characteristics of materials has advanced to a state where better measurements of radiation damage can be determined. To understand the response of a material to neutron exposure, it is necessary to calculate the

damage-energy delivered to the material.

The Rotating Target Neutron Source (RTNS-I) facility consists of a high intensity neutron source and a rotating, water-cooled target (see Fig. 1). The insulated core transformer (ICT)-accelerator used in RTNS-I presently delivers a 15- to 25-mA deuteron beam collimated to a diameter of 1.6 cm. Most of the current is concentrated to within less than half this diameter. 15-MeV neutrons are produced by deuteron

bombardment of the tritium absorbed in the titanium target. The target is rotated at high speeds and is water-cooled to dissipate the large amount

of power in the deuteron beam. Table 1 summarizes the main parameters of RTNS-I and also of RTNS-II, which will become operational about July 1, 1978.

Fig. 1. Target system of RTNS-I.

Table 1. Lawrence Livermore Laboratory 14-MeV neutron sources.

Parameter	RTNS-I	RTNS-II	
		Initial operation	Upgraded operation
Supply, mA,kV	60,400	300,500	600,500
Target current, mA	20	40-160	400
Beam diameter, cm	0.6	0.6-1.0	1.0
Power density, kW/cm ²	30	60-80	200
Target diameter, cm	23	46-70	70
Rotation speed, rpm	1100	5000-10 000	10 000
Source strength, 10 ¹² n/sec	5	10-40	100
Small sample flux, 10 ¹² n/cm ² sec	2	4-16	?
Target lifetime, hr (20% yield drop)	100	100	?

Damage Energy Calculation

The computer program input requires material cross-section and angular distribution data for a particular material, along with the incident neutron spectrum of interest. The energy-dependent cross-section and elastic distribution data are taken from the *Livermore Evaluated Neutron Cross-Section Library*.¹ These data are also used for LLL neutron transport calculations. The neutron spectrum and group boundary structure is defined by the user (e.g., see Fig. 2). Isotopic data

Fig. 2. Neutron spectrum of RTNS-I.

and the threshold energy for displacement in the primary event are also required as input data. Linear interpolation is used in matching input flux, cross sections, and energy values and also in subsequent calculations.

The calculative procedure basically utilizes the input data, com-

bined with classical and relativistic mechanics, to obtain the primary-recoil energy and damage-energy spectra for the material of interest. The main nuclear reactions considered are elastic, (n, n') , $(n, 2n)$, and $(n, +)$. For RTNS, the (n, γ) reaction is not important in damage production and is not included. For elastic reactions, we use input angular distributions, and for non-elastic reactions we assume isotropic scattering. For nonelastic reactions in which the secondary particles consist of one or more neutrons, the energy distribution of the secondary particles is chosen from a nuclear temperature plus a pre-equilibrium component. Only the first particle out is considered. For outgoing charged particles, we assume that the energy spectrum is Gaussian, centered at the Coulomb energy, dropping to 1% of the maximum value for zero-emitted energy.

The following is a summary of the principal steps in the calculations:

1. The input spectrum is plotted.
2. The input flux is partitioned, and average energies and cross sections are calculated for each group. All neutrons within a group are now assumed to be of the calculated average energy and cross section.

3. A matrix containing flux-weighted cross sections for each reaction type and each neutron energy group is calculated.
4. The normalized "primary knock-on atom" (PKA) spectrum for elastic recoils is calculated for each group.
5. The nuclear temperature is interpolated from tabular values² (see Fig. 3).

Fig. 3. Nuclear temperature as a function of atomic mass.

6. The normalized PKA spectrum resulting from inelastic collisions is calculated and plotted for each group.
7. The normalized PKA spectrum for charged-particle recoils

is calculated and plotted for each group.

8. All spectra are collapsed into a single primary-recoil spectrum. Plots are made of the resulting primary-recoil spectrum as well as the normalized integral of the spectrum.
9. The primary recoil spectrum is now converted to a damage-energy spectrum by using theoretical expressions derived (by Lindhard *et al.*,³ and Robinson⁴) for damage efficiency of creating atom displacements in materials. Plots are made of the damage-energy spectrum as well as the normalized integral of the spectrum.

The integral of the damage-energy spectrum is a measure of the damage effectiveness of the input neutron spectrum. This parameter is proportional to the rate of atom displacement and is the product of (a) the cross section for producing a primary recoil and (b) the average damage-energy per primary recoil. Table 2 lists the calculated results of the RTNS-I neutron spectrum on aluminum, iron, copper, and niobium. The spectrum-averaged cross sections listed were calculated from the LLL cross-section library data.¹

Table 2. Spectrum-averaged cross sections for RTNS-I (figures in barns unless otherwise noted).

Nuclear reaction	Aluminum	Iron	Copper	Niobium
Elastic	6.5×10^{-1}	1.1×10^0	1.5×10^0	2.2×10^0
(n, n')	6.6×10^{-1}	7.8×10^{-1}	5.1×10^{-1}	4.1×10^{-1}
(n, 2n)	1.0×10^{-1}	4.7×10^{-1}	7.3×10^{-1}	1.2×10^0
(n, n'p)	—	—	1.3×10^{-1}	—
(n, n'α)	—	—	—	2.6×10^{-3}
(n, p)	7.1×10^{-2}	1.1×10^{-1}	7.6×10^{-2}	4.0×10^{-2}
(n, d)	3.0×10^{-2}	—	—	—
(n, t)	6.0×10^{-4}	—	—	—
(n, α)	1.2×10^{-1}	2.9×10^{-2}	2.5×10^{-2}	9.2×10^{-3}
(n, γ)	2.1×10^{-4}	6.2×10^{-5}	5.6×10^{-4}	7.8×10^{-4}
Total	1.63	2.50	2.94	3.93
σ _{recoil}	1.63	2.50	2.94	3.92
Damage energy, barns - keV	162	272	277	263

Limitations and Discussion

The computer program described here can be applied to most neutron spectra with the following limitations:

- The present omission of (n, γ) limits application to cases where this reaction is not important.
- The Lindhard expression used for electron-excitation losses is only appropriate for pure metals.
- The nonelastic and Lindhard theories used are invalid for elements lighter than aluminum.

A number of safeguards built into

the program protect the user from some of the more common pitfalls. Messages are printed out, and in some cases the calculation is stopped when the following problems are discovered:

- The material of interest does not match the cross section and angular distribution input data.
- The defined group boundaries do not fall within the input neutron spectrum.
- The energy entries are not sequential.
- The input data exceeds the dimensioned storage space.

- Either the angular or the energy distributions fail to integrate to one.

Also, a warning is printed if the user attempts calculations that are outside the mass range where the nuclear temperature model is appropriate.

In addition to the above, an option is available for determining the amount of information output. When other input error is suspected, this option allows the user to request the maximum output for checking various stages of the calculation.

Calculations were made for the RTNS-I neutron spectrum on aluminum, titanium, vanadium, iron, nickel, copper, zirconium, niobium, molybdenum, silver, tin, tantalum, tungsten, gold, and lead. Table 3 summarizes our damage-energy calculations and compares them to similar calculations made by others.⁵⁻⁹ The remaining illustrations - Figs. 4 through 63 - show graphical computer output for:

- The primary recoil spectrum both in log-linear (e.g., Fig. 4) and log-log form (e.g., Fig. 5).

Table 3. Summary of results of damage-energy calculations and comparison with results of others (damage energy given in barns - keV).

Element	Data source					
	This work	Doran and Yoshikawa, ⁵ Eds.	Parkin <u>et al.</u> ⁶	Roberto <u>et al.</u> ⁷	Parkin and Goland ⁸	Omar <u>et al.</u> ⁹
Al	163	189	164		173	
Ti	259					
V	247		237			
Fe	272					278
Ni	312	263				254
Cu	277	273		301	272	267
Zr	236	240				200
Nb	263		273	266	274	266
Mo	246					
Ag	228					
Sn	229					
Ta	212					
W	201	201				
Au	183			212	194	188
Pb	193	210				

- The normalized integral of the recoil spectrum (e.g., Fig. 6).
- The normalized integral of the damage energy spectrum (e.g., Fig. 7).

Acknowledgment

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Fig. 4. The primary recoil spectrum (semi-log).

Fig. 5. The primary recoil spectrum (log-log).

Fig. 6. The normalized integral of the recoil spectrum.

Fig. 7. The normalized integral of the damage energy spectrum.

Fig. 8. The primary recoil spectrum (semi-log).

Fig. 9. The primary recoil spectrum (log-log).

Fig. 10. The normalized integral of the recoil spectrum.

Fig. 11. The normalized integral of the damage energy spectrum.

Fig. 12. The primary recoil spectrum (semi-log).

Fig. 13. The primary recoil spectrum (log-log).

Fig. 14. The normalized integral of the recoil spectrum.

Fig. 15. The normalized integral of the damage energy spectrum.

Fig. 16. The primary recoil spectrum (semi-log).

Fig. 17. The primary recoil spectrum (log-log).

Fig. 18. The normalized integral of the recoil spectrum.

Fig. 19. The normalized integral of the damage energy spectrum.

Fig. 20. The primary recoil spectrum (semi-log).

Fig. 21. The primary recoil spectrum (log-log).

Fig. 22. The normalized integral of the recoil spectrum.

Fig. 23. The normalized integral of the damage energy spectrum.

Fig. 24. The primary recoil spectrum (semi-log).

Fig. 25. The primary recoil spectrum (log-log).

Fig. 26. The normalized integral of the recoil spectrum.

Fig. 27. The normalized integral of the damage energy spectrum.

Fig. 28. The primary recoil spectrum (semi-log).

Fig. 29. The primary recoil spectrum (log-log).

Fig. 30. The normalized integral of the recoil spectrum.

Fig. 31. The normalized integral of the damage energy spectrum.

Fig. 32. The primary recoil spectrum (semi-log).

Fig. 33. The primary recoil spectrum (log-log).

Fig. 34. The normalized integral of the recoil spectrum.

Fig. 35. The normalized integral of the damage energy spectrum.

Fig. 36. The primary recoil spectrum (semi-log).

Fig. 37. The primary recoil spectrum (log-log).

Fig. 38. The normalized integral of the recoil spectrum.

Fig. 39. The normalized integral of the damage energy spectrum.

Fig. 40. The primary recoil spectrum (semi-log).

Fig. 41. The primary recoil spectrum (log-log).

Fig. 42. The normalized integral of the recoil spectrum.

Fig. 43. The normalized integral of the damage energy spectrum.

Fig. 44. The primary recoil spectrum (semi-log).

Fig. 45. The primary recoil spectrum (log-log).

Fig. 46. The normalized integral of the recoil spectrum.

Fig. 47. The normalized integral of the damage energy spectrum.

Fig. 48. The primary recoil spectrum (semi-log).

Fig. 49. The primary recoil spectrum (log-log).

Fig. 50. The normalized integral of the recoil spectrum.

Fig. 51. The normalized integral of the damage energy spectrum.

Fig. 52. The primary recoil spectrum (semi-log).

Fig. 53. The primary recoil spectrum (log-log).

Fig. 54. The normalized integral of the recoil spectrum.

Fig. 55. The normalized integral of the damage energy spectrum.

Fig. 56. The primary recoil spectrum (semi-log).

Fig. 57. The primary recoil spectrum (log-log).

Fig. 58. The normalized integral of the recoil spectrum.

Fig. 59. The normalized integral of the damage energy spectrum.

Fig. 60. The primary recoil spectrum (semi-log).

Fig. 61. The primary recoil spectrum (log-log).

Fig. 62. The normalized integral of the recoil spectrum.

Fig. 63. The normalized integral of the damage energy spectrum.