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TITLE: CALCULATIONS FOR ISOTOPICALLY-TAILORED CERAMICS IN FISSION AND FUSION REACTORS

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CALCULATIONS FOR ISOTOPICALLY-TAILORED CERAMICS IN FISSION AND FUSION REACTORS

by

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ABSTRACT

Information and understanding of the response of a ceramic at dpa and gas production rates near those expected at the first wall of a fusion reactor can be obtained by an experiment in a fission reactor to irradiate an isotopically tailored sample of the ceramic. To aid in the design of such an experiment, we have made calculations to determine the amount of ^{15}N and ^{17}O needed in $Si_3Al_3O_3N_5$ and ^{17}O needed in Al_2O_3 to simulate the behavior of these ceramics in the first wall of the STARFIRE fusion reactor by exposure in the HFIR reactor at Oak Ridge National Laboratory. The calculations were performed using a code developed at Hanford Engineering Development Laboratory, and the gas production and damage nuclear data needed were produced with a Los Alamos code. Although the damage data are more appropriate for metals, it is assumed that the comparison of the gas-to-damage ratios in the two reactors is valid. Calculations indicate that 57% ^{17}O and 90.6% ^{15}N in sialon and 17.9% ^{17}O in alumina would be adequate for the simulation.

INTRODUCTION

A necessary first step in a program to develop ceramics for applications in which the materials are exposed to high fluences of fusion neutrons is to determine the effects of the neutron irradiation at approximately correct dpa and gas production rates. Because the actual fluences needed for testing the materials are unavailable in any existing reactor, a simulated exposure must be made in a fission reactor. This can be done by isotopically tailoring the ceramic so that the ratio of the gas-production to displacements-per-atom of the tailored sample irradiated in the fission reactor would equal that for a normal sample in the first wall of a fusion assembly. $Si_3Al_3O_3N_5$ (sialon) and Al_2O_3 (alumina) are the ceramics that have been chosen for an irradiation experiment in the high

Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory. The purpose of this report is to describe calculations for determining the fractional content of the isotopes ^{15}N and ^{17}O in sialon and ^{17}O in alumina needed to simulate the behavior of normal sialon and alumina in the first wall of the STARFIRE fusion reactor design by an irradiation experiment in the PTP (peripheral test position, near the central plane) zone of HFIR.

Calculational Method

The calculations were done with the REAC code system,[1] which was designed to calculate activation rates, dose rates, delayed photon production yields, transmutation yields, and reaction rates for specific reactions for a variety of materials in many different environments and for various residence and cooling times. The system consists of a driver code, flux libraries, cross-section libraries, a materials library, and a decay library. Although in our calculations we only used this versatile code for flux-averaging over the reactions, it was chosen for its "user-friendly" input, availability of HFIR PTP and STARFIRE first wall spectra in the flux library, availability of damage and gas production data in the cross-section library, and ease with which the material library could be changed for running problems with different isotopic fractions.

The isotopic contents of normal sialon and alumina are given in Table I. Note, in particular, that the elemental fractions in both ceramics do not differ widely, and also the atomic weights of the constituents differ by no more than a factor of two. This is important, as it is the opinion of at least one expert[2] that, under these conditions, the averaging over the constituents for dpa, as performed by REAC using the damage cross sections generated by the NJOY code,[3] is approximately valid for ceramics even though the underlying theory[4] is more appropriate for metals. Furthermore, inaccuracies due to approximations tend to cancel in the ratio comparisons used in this work.

Nuclear Data

The nitrogen and oxygen isotopic reactions contributing to hydrogen and helium gas production, for which cross section data are available in the REAC library CROSS, are listed in Table II. These were generated by the NJOY code system using ENDF/B-V[5] basic nuclear data as input. The various cross sections were summed by NJOY so that CROSS contains specific H and He production cross sections for each isotope. These are compared with each other and with the HFIR

PTP and STARFIRE first wall spectra in Figs. 1a, 1b, and 2a, 2b. Note from the threshold energies of the cross sections shown in these figures that the H-production can be most easily adjusted with the $^{15}N/N$ ratio; whereas, both the $^{15}N/N$ and $^{17}O/O$ ratios can be used to adjust the He-production.

The dpa data from our version of CROSS for Si, Al, O, and N and the HFIR PTP and STARFIRE first wall spectra are compared in Figs. 3a and 3b. The units for these cross sections are keV-b, so they may be more properly termed "displacement damage-energy" cross sections rather than dpa cross sections. The rather sudden increase of three orders of magnitude in the oxygen data at about 60 eV led us to suspect an error (e.g., in units--eV vs keV) in the CROSS library data, so we made a comparison with damage data generated by Greenwood and Smither using the SPECTER code[6]. NJOY and SPECTER use similar methods for generating damage data and earlier comparisons[4] have shown that the two codes give comparable results. Our comparisons for Si, Al, O, and N are shown in Figs. 4a and 4b. Again note the large discrepancy in the oxygen data above 60 eV. We, therefore, concluded that these data were indeed in error by a factor of 1000 in the CROSS library and made corrections accordingly. The data in the revised library are compared with the SPECTER data in Fig. 5, and now the agreement is quite good.

RESULTS

REAC calculational results are shown in Tables III and IV. The units of the values given in the tables for the gas/damage ratios are relative but comparable for all cases. Exposure times and power levels cancel out in the ratios, and the conversion of displacement damage-energy to displacement damage (DPA) is ignored because the conversion factors for the several constituents in each ceramic are about the same. According to Ref. 6, this factor is $0.8/2E_d$, where values for E_d, the Linhard cutoff energy required to displace the atom, are given in the reference. These assumed to be are 25, 27, 30, and 30 eV for Si, Al, O, and N, respectively.

As indicated in Table III, the ^{15}N content of the sialon was mainly adjusted by the H/damage ratio; whereas, the ^{17}O content was adjusted with the He/damage ratio. The final isotopic percentages for simulation of the sialon are 90.6% and 57.0% for ^{15}N and ^{17}O, respectively.

In the case of alumina, the results for which are shown in Table IV, only the He/damage ratios can be matched since, as indicated above, the H/damage

ratio is practically impossible to adjust with ^{17}O. Note that the simulation is achieved with 17.9% ^{17}O.

Although the results reported in Tables III and IV were obtained using the revised oxygen damage cross sections, the calculations were initially done using the incorrect data. These initial results indicated 92% ^{15}N and 50% ^{17}O contents for the sialon simulation and an 18% ^{17}O content for the alumina simulation which show a rather remarkable insensitivity of these calculations to a factor of 1000 change in the oxygen dpa data. The integral dpa cross sections in the HFIR PTP and STARFIRE first wall were in fact very nearly the same, differing by factors of only 1.5 for sialon and 1.2 for alumina. Thus, we can conclude that the approximations we made in these calculations are valid and that the results are reliable.

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Table I

Isotope Fractions in Normal $Si_3Al_3O_3N_5$ and Al_2O_3

Isotope	Sialon Fractions	Alumina Fractions
^{14}N	3.558×10^{-1}	--
^{15}N	1.320×10^{-3}	--
Total N	0.3571	--
^{16}O	2.138×10^{-1}	5.986×10^{-1}
^{17}O	8.000×10^{-5}	2.000×10^{-4}
^{18}O	4.300×10^{-4}	1.200×10^{-3}
Total O	0.2144	0.6000
^{27}Al	2.143×10^{-1}	4.000×10^{-1}
Total Al	0.2143	0.4000
^{28}Si	1.976×10^{-1}	--
^{29}Si	1.001×10^{-2}	--
^{30}Si	6.640×10^{-3}	--
Total Si	0.2142	--

Table II

Reactions in CROSS Library Contributing to Gas Production

H Production

^{14}N Reactions	^{15}N Reactions
$^{14}N(n,np)^{13}C$	$^{15}N(n,np)^{14}C$
$^{14}N(n,nd)^{12}C$	$^{15}N(n,np)^{13}C$
$^{14}N(n,nt)^{11}C$	$^{15}N(n,nt)^{12}C$
$^{14}N(n,p)^{14}C$	$^{15}N(n,p)^{15}C$
$^{14}N(n,d)^{13}C$	$^{15}N(n,d)^{14}C$
$^{14}N(n,t)^{12}C$	$^{15}N(n,t)^{13}C$
$^{14}N(n,2p)^{13}B$	$^{15}N(n,2p)^{14}B$
^{16}O Reactions	**^{17}O Reactions**
$^{16}O(n,np)^{15}N$	$^{17}O(n,np)^{16}N$
$^{16}O(n,nd)^{14}N$	$^{17}O(n,nd)^{15}N$
$^{16}O(n,nt)^{13}N$	$^{17}O(n,nt)^{14}N$
$^{16}O(n,p)^{16}N$	$^{17}O(n,p)^{17}N$
$^{16}O(n,d)^{15}N$	$^{17}O(n,d)^{16}N$
$^{16}O(n,t)^{14}N$	$^{17}O(n,2p)^{16}C$
$^{16}O(n,2p)^{15}C$	

He Production

^{14}N Reactions	^{15}N Reactions
$^{14}N(n,n\alpha)^{10}B$	$^{15}N(n,n\alpha)^{11}B$
$^{14}N(n,\alpha)^{11}B$	$^{15}N(n,n^4He)^{12}B$
$^{14}N(n,2\alpha)^{7}Li$	$^{15}N(n,\alpha)^{12}B$
$^{14}N(n,^4He)^{12}B$	
^{16}O Reactions	**^{17}O Reactions**
$^{16}O(n,n\alpha)^{12}C$	$^{17}O(n,n\alpha)^{13}C$
$^{16}O(n,n\alpha)^{13}C$	$^{17}O(n,n^4He)^{14}C$
$^{16}O(n,^4He)^{14}C$	$^{17}O(n,\alpha)^{14}C$
$^{16}O(n,\alpha)^{13}C$	

Table III

Gas/Damage Ratio Calculations for $Si_3Al_3O_3N_5$

Reactor/Region	$^{15}N/N$	$^{17}O/O$	H/Damage	He/Damage
STARFIRE/1st Wall	Normal	Normal	94.9	61.8
HFIR/PTP	Normal	Normal	998.5	25.7
HFIR/PTP	0.87	0.55	131.7	60.5
HFIR/PTP	0.92	0.55	81.7	59.3
HFIR/PTP	0.91	0.55	91.5	59.4
HFIR/PTP	0.908	0.55	93.7	59.5
HFIR/PTP	0.92	0.50	70.4	55.6
HFIR/PTP	0.908	0.50	93.7	54.6
HFIR/PTP	0.906	0.57	95.7	61.8

Table IV

Gas/Damage Ratio Calculations for Al_2O_3

Reactor/Region	$^{15}N/N$	$^{17}O/O$	H/Damage	He/Damage
STARFIRE/1st Wall	---------	Normal	28.6	58.0
HFIR/PTP	---------	Normal	1.4	4.7
HFIR/PTP	---------	0.55	1.4	171.4
HFIR/PTP	---------	0.17	1.4	55.5
HFIR/PTP	---------	0.26	1.4	83.3
HFIR/PTP	---------	0.179	1.4	58.8

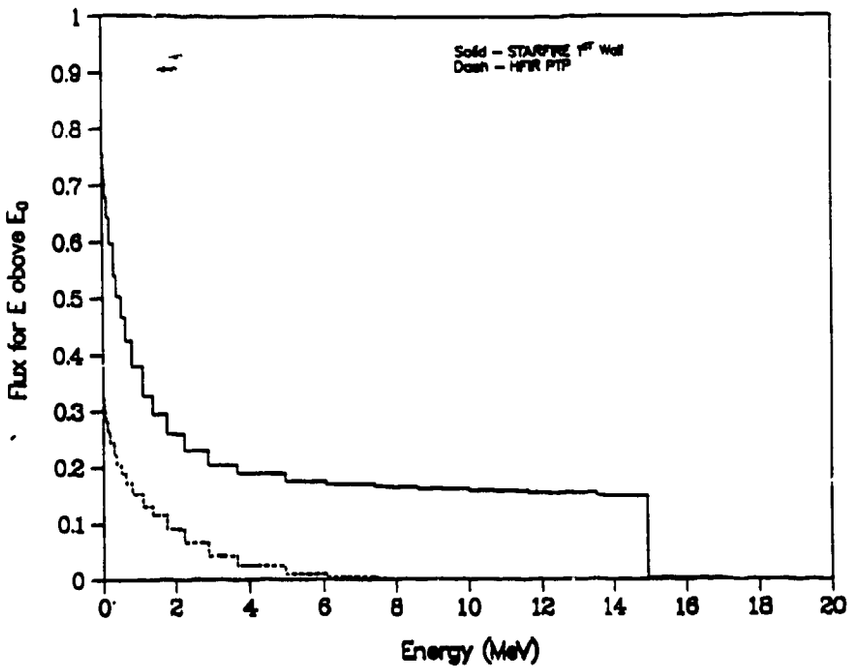

Fig. 1a. Comparison of STARFIRE first wall and HFIR PTP fractional cumulative fluxes.

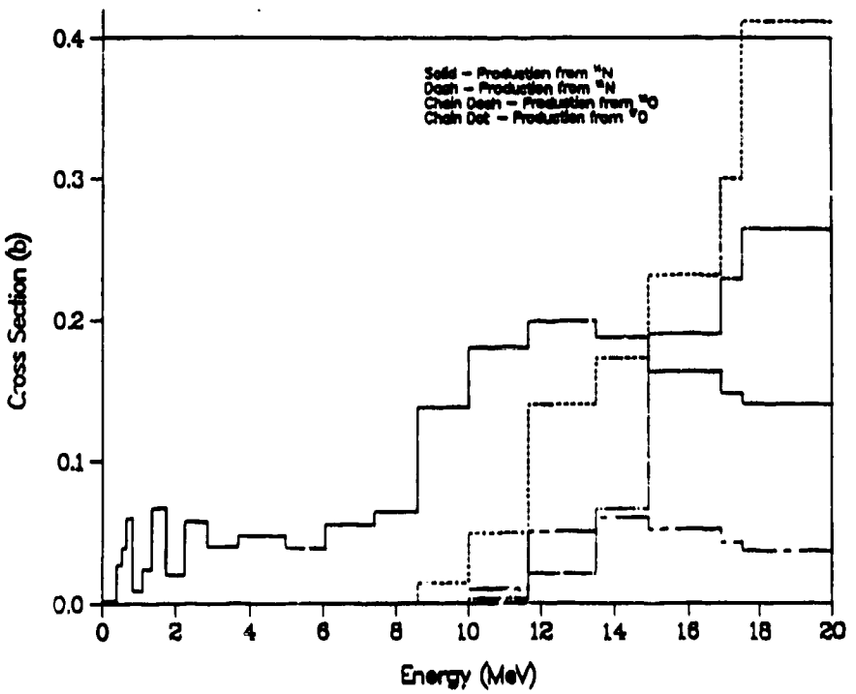

Fig. 1b. Comparison of H production by isotope.

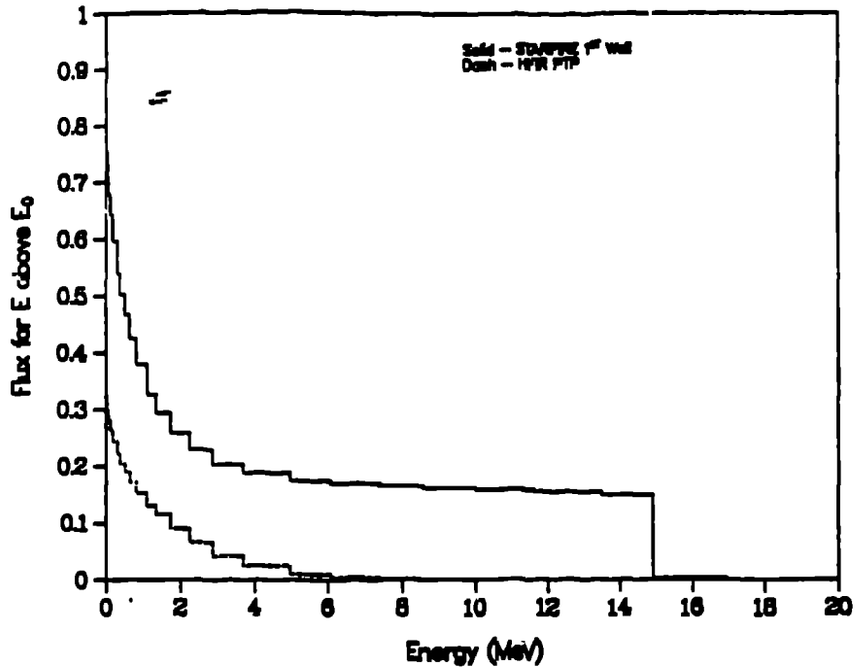

Fig. 2a. Comparison of STARFIRE first wall and HFIR PTP fractional cumulative fluxes.

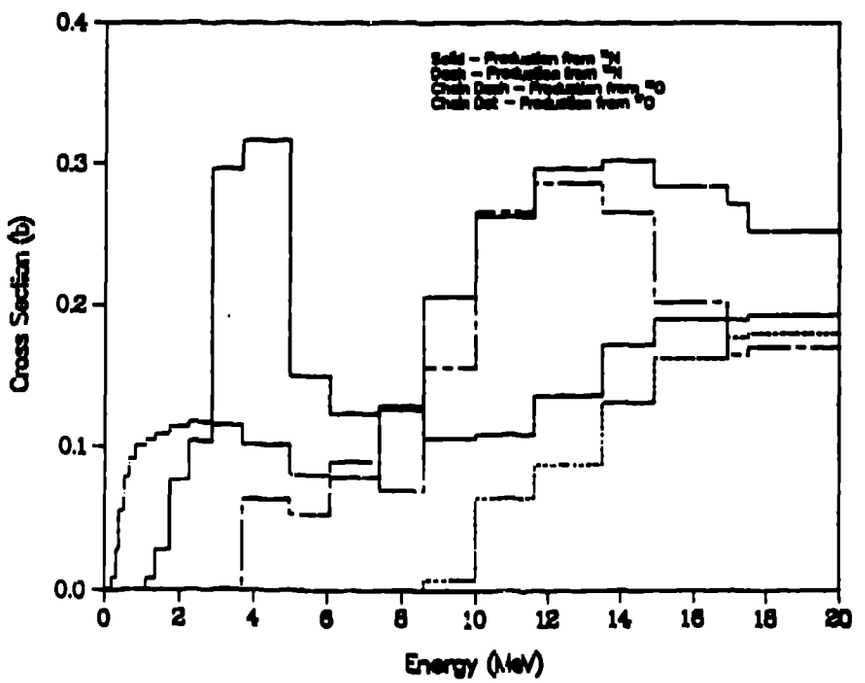

Fig. 2b. Comparison of He production by isotope.

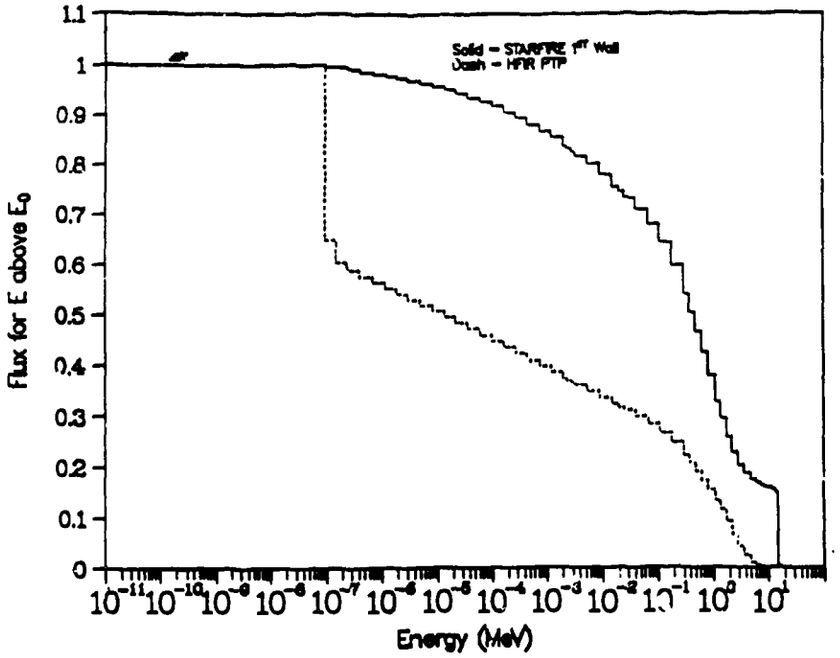

Fig. 3a. Comparison of STARFIRE first wall and HFIR PTP fractional cumulative fluxes.

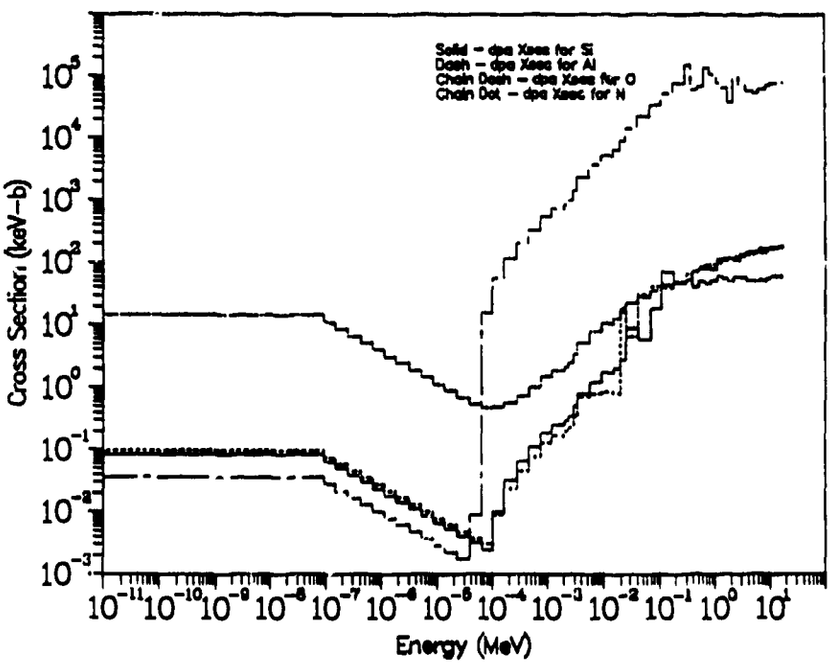

Fig. 3b. Comparison of Si, Al, O, and N dpa cross sections.

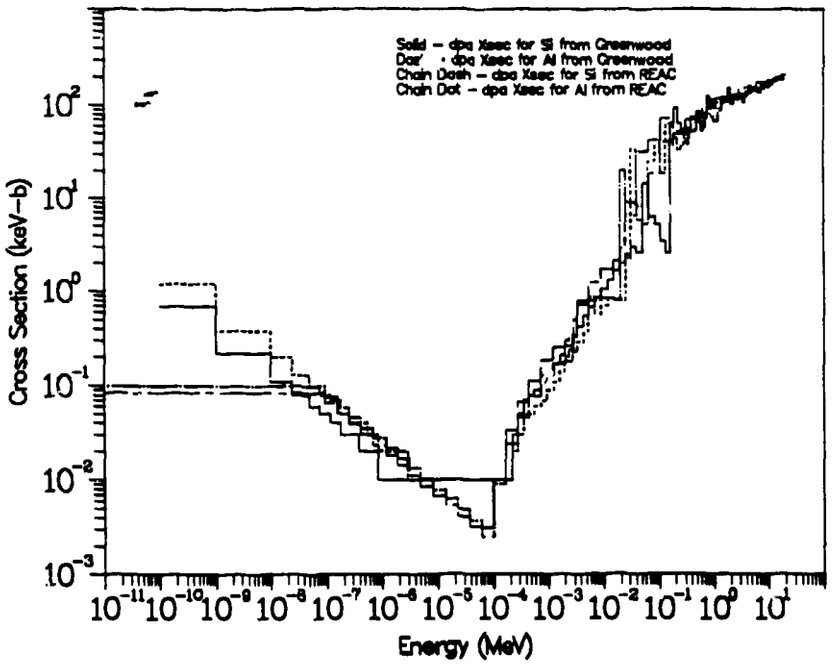

Fig. 4a. Comparison of Si and Al dpa cross sections - Greenwood/REAC.

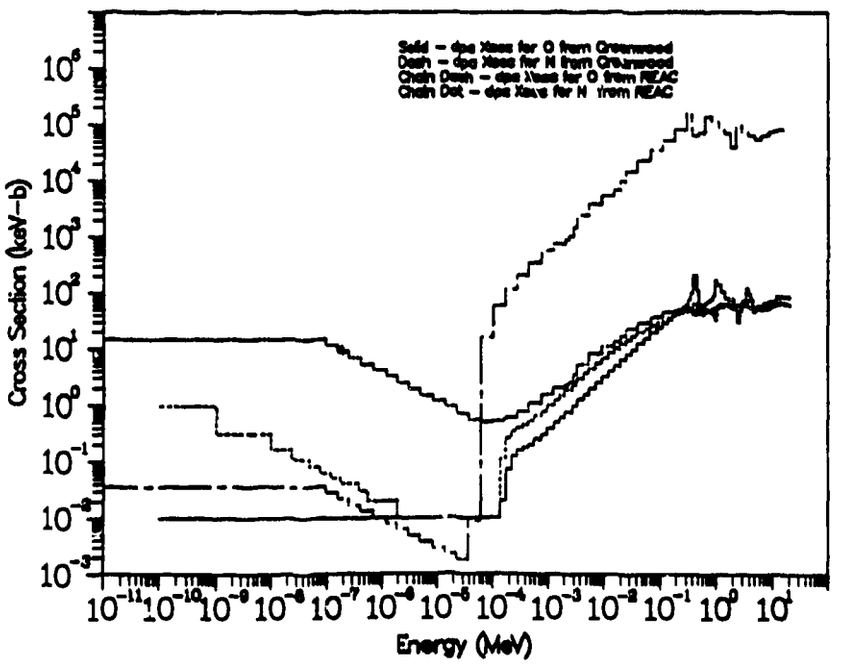

Fig. 4b. Comparison of O and N dpa cross sections - Greenwood/REAC.

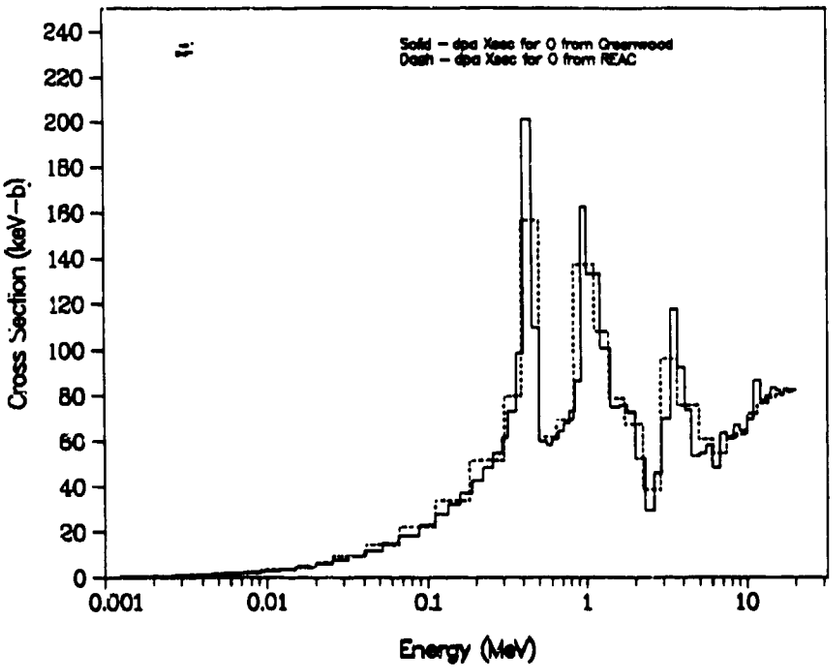

Fig. 5. Comparison of O dpa cross sections - Greenwood/REAC.