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A Review of Activation Cross Sections in the ENDF/B-VI General Purpose Files for Cr, Fe, Ni, Cu, and Pb

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ABSTRACT

Isotopic evaluations for ^{50,52,53,54}Cr, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu, and ^{206,207,208}Pb are included in ENDF/B-VI for the first time. These general purpose files, all by the ORNL evaluation group, include many activation cross sections. In this review, the 34 activation reactions for these materials in the priority-I CSEWG list were checked for their presence and contents in the general purpose files. These cross sections are reviewed in terms of the experimental data base and the evaluation methods. Most of them have been significantly improved over ENDF/B-V through the improved data base and the use of advanced codes such as SAMMY for resonance analysis, GLUCS for handling ratio data and covariances, and TNG for cross-section shape and for extracting individual cross sections from the measured particle spectrum.

1. INTRODUCTION

In producing the ENDF/B-VI general purpose files with limited man power, not enough attention has been paid to some "small" cross sections and cross sections of isotopes with "low" natural abundance. However, for activation analysis these small cross sections can be important. This timely NEANDC meeting has drawn our attention to the importance of activation cross sections, particularly those needed for fusion reactor design. Our first response was to check and see if all of the priority-I activation cross sections in the May 1984 CSEWG list[1] are included in the files we are responsible for, leading to plans for some additional work. The second purpose is to delineate adequate and inadequate evaluations, hopefully resulting in recommendations either for adoption in a new Activation File or for additional evaluations and/or measurements. To this goal, the evaluation methods and the data base are summarized.

The priority-I list[1] for ENDF/B-VI activation cross sections was checked against the high priority fusion activation data table of Cheng[2] to make sure that the fusion data needs for activation cross sections are also covered in this review. In addition, one reaction from the priority-II list,[1] ^{206}Pb(n,2n)^{205}Pb, is also included. The high-priority need for this cross section is based on the work of Forrest and Endacott[3] in which it is shown that, for a neutron spectrum in the first wall of a DEMO fusion reactor, the production of ^{205}Pb in natural Pb by ^{206}Pb(n,2n) is 200 times greater than by ^{204}Pb(n,γ). Since the latter is included in the priority-I list and ^{205}Pb has a half life of 14 million years, it is desirable to upgrade ^{206}Pb(n,2n) to priority I. The reactions ^{58}Fe(n,γ) and ^{63}Cu(n,2n) are also included in this review as they are commonly used dosimeters for fission and fusion applications.[1,2] The total number of reactions included in this review is thus 37.

The evaluation methods and data base are summarized in Sect. 2. The activation cross sections being added to the presently approved (April 1989) ENDF/B-VI general purpose files mentioned above are listed in Sect. 3, along with conclusions from our preliminary investigation. Section 4 summarizes the adequacy of each reaction based on the experimental data available and the sophistication of the evaluation methods used.

2. SUMMARY OF EVALUATION METHODS AND DATA BASE

The evaluation methods chosen depend on the type of reaction and on the number and quality of data available. On these basis, we group our review as follows. The evaluation method and data base for each individual activation cross section are summarized in Table 1 (see Sect. 4).

SAMMY FOR RESONANCE ANALYSIS

SAMMY,[4] an R-matrix code based on the Reich-Moore formalism and the Bayes' Equations, was used for the resonance region of ^{58}Ni. The analysis[5] was based on measured cross sections for total and capture, and the angular distributions of elastic scattering. The resulting ^{58}Ni(n,γ) cross section is of the highest quality currently achievable.

MUGHABGHAB RESONANCE PARAMETERS

The other (n,γ) cross sections for which extensive SAMMY analysis was not performed have also been significantly improved over ENDF/B-V because the experimental information compiled by Mughabghab[6] on neutron and gamma-ray widths, which were used in the evaluations, has vastly increased since the earlier edition. For example, the number of resonances in ^{58}Fe has increased from 6 in ENDF/B-V to 67 in ENDF/B-VI. Energies and widths of distant resonances were generated using SAMMY to account for thermal cross sections and the background in the total cross sections. The point cross sections for capture were checked with experimental data if available for determining the background cross sections.

A weakness in most of the (n,γ) evaluations covered in this review exists around $0.5 < E_n < 1.0$ MeV, the upper energy of the resonance region in which resonances become unresolved, energy-averaged experimental data are scarce, and accurate statistical model calculations are difficult. Experimental data are most needed in this energy range to establish the background cross sections near the upper end of the resolved resonance region and to provide a point of normalization for calculated values for the higher energy range.

GLUCS FOR RATIO DATA AND COVARIANCES

GLUCS,[7] a generalized least-squares code for updating evaluated cross sections with new data (including ratios and covariances), was used for the dosimetry cross sections ^{54,56}Fe(n,p), ^{58}Ni(n,p), ^{63,65}Cu$(n,2n)$, and ^{63}Cu(n,α), all of which were linked by ratio data. The code was upgraded to read and write new ENDF/B-VI covariance format (LB = 8 for positive definiteness of the covariance matrix). Recent ENDF/B-VI data[8] for ^{235,238}U(n,f), an evaluation of ^{27}Al(n,α) by Vonach,[9] and an evaluation of ^{32}S(n,p) by Divadeenam[10] were used as standards for handling ratios. Other details are the same as reported earlier.[11,12] Cross sections of ^{27}Al(n,p) and ^{46,47,48}Ti(n,p), not covered in this review, were also linked to the others by ratio data in the present work.

For this group of reactions analyzed with GLUCS, improvements over ENDF/B-V are mainly in the resulting covariances which are more credible and mathematically sound. Experimental data are believed adequate for activation analysis and probably so for dosimetry purposes. The most difficult (and uncertain) part of this work was to extract covariance information from the experimental papers.

TNG FOR PREDICTION

TNG,[13] a multistep Hauser-Feshbach/preequilibrium model code, was used for calculating all non-resonance cross sections required for coupled neutron and gamma transport calculations. In general, optical model and level density parameters were adjusted to obtain the best simultaneous overall fit to minimize the size of normalization of each reaction cross section to experimental data. Reaction cross sections not dominated by statistical reaction mechanisms, such as (n,d), (n,t), and $(n,{}^3\mathrm{He})$, are evaluated by the empirical methods described below.

The statistical model codes, such as TNG, are particularly useful for extracting the cross section of a reaction having a long-lived daughter from the measured particle spectrum. Due to the long half life of the product nuclide, the reaction cross section cannot be easily measured by activation methods. However, the measured particle spectrum often includes more than one reaction. The statistical model code can be used to fit the measured spectrum and separate the cross section of several combined reactions into individual ones. An example, the proton spectrum of the $^{63}\mathrm{Cu}(n,px)$ reaction for $E_n = 14.8$ MeV, is shown in Fig. 1. Due to the long half life (100 years) of the daughter nuclide, the (n,p) cross section has not been measured directly. The available proton spectrum[14] is composed mainly of (n,p) and (n,np) and the model calculation was used to separate the two reaction cross sections. Note that in the model calculation, as seen in Fig. 1, the (n,np) and (n,pn) are separate channels; (n,np) results from a proton competition with gamma rays in the (n,n') channel and (n,pn) comes from a neutron competition with gamma rays in the (n,p) channel. In this case, knowledge about the gamma-ray strength function plays a role. Since the (n,p) part of the proton spectrum is in the high-energy end of the total proton spectrum, the pre-equilibrium effect is also important.

For the $^{50}\mathrm{Cr}(n,2n)$ reaction, the available data cover a large part of the energy region but the shape of the cross section defined by the data differs from the calculated shape. In this case, it was decided to use the data directly.

INTEGRAL DATA

Integral data have not been used systematically in the present differential evaluations but have been used to guide evaluation of the $^{60}\mathrm{Ni}(n,p)^{60}\mathrm{Co}$ cross section for which large discrepancies in the differential data exist. Two sets[15,16] of data have 50% difference in the important energy range between 7 and 13 MeV. We chose the lower data set[16] for better agreement with the integral value measured for a $^{252}\mathrm{Cf}$ benchmark field by Mannhart.[17] The integral values calculated from ENDF/B-V and ENDF/B-VI are 3.44 mb and 2.61 mb, respectively, while the measured one is 2.39 ± 0.13 mb.

14-MEV SYSTEMATICS OR DATA

Systematics of Qaim et al.[18] for the (n,d), (n,t), and $(n,{}^3\mathrm{He})$ cross sections at 14 MeV were used where measured data are not available. The shape of (n,d) and (n,t) cross sections were taken from the TNG calculation for (n,p), adjusted for threshold differences, and that of $(n,{}^3\mathrm{He})$ from (n,α). For heavy targets such as Pb, the (n,p) and (n,α) cross sections are very small and since the model calculations become unreliable for small cross sections, systematics were used for normalization where data are not available. A single experimental datum near 14 MeV was treated in the evaluation process in the same manner.

3. EVALUATIONS IN PROGRESS

A general purpose file for ^{204}Pb, omitted due to its low natural abundance, is needed. Not only would the file contain the three priority-I activation cross sections, ^{204}Pb(n,γ), (n,p), and $(n,2n)$, the presence of a general purpose file for this isotope would also properly account for the capture cross section for natural Pb in the energy region for E_n between 2 to 10 keV. In this energy range, the 1% ^{204}Pb contributes 30% to the capture cross section for natural Pb.[19] An effort is being made to add a ^{204}Pb evaluation to complete the isotopic evaluations for Pb.

Other priority-I cross sections being added to the presently approved (not yet released) ENDF/B-VI general purpose files are ^{50}Cr$(n,d)^{49}$V, ^{54}Fe$(n,d)^{53}$Mn, ^{65}Cu$(n,t)^{63}$Ni, ^{61}Ni$(n,2p)^{60}$Fe, and ^{206}Pb$(n,nd)^{204}$Tl.

Preliminary investigations for the above eight activation cross sections have been made. They are included in the summary table below as if completed.

4. SUMMARY TABLE

Table 1 lists the activation reactions, induced radionuclides and their half lives, and comments. The comments have the following 9 categories in order of the quality of the available data and the evaluation methods.

1. Sufficient data , GLUCS analysis, Covariances: 6 reactions
2. Sufficient data, SAMMY analysis: 1 reaction
3. Sufficient data, TNG calculation: 7 reactions
4. Curve drawn through data: 1 reaction
5. Conflicting data, integral data used to guide evaluation: 1 reaction
6. Insufficient data, TNG calculation: 4 reactions
7. Mughabghab parameters and SAMMY: 7 reactions
8. 14-MeV systematics or data: 7 reactions
9. TNG prediction only: 3 reactions

These comments are self-explanatory, though their assignments are somewhat subjective. For example "insufficient data, TNG calculation" simply means that the available data cover only a "small" energy range and the shape of the cross section was largely determined by theory.

Among the three that depended on "TNG prediction only", the cross section of ^{60}Ni$(n, 2n)^{59}$Ni will need experimental confirmation because (1) the evaluated cross section is relatively large (350 mb at 14 MeV), (2) according to Forrest and Endacott,[3] this reaction is nearly equal in importance as ^{58}Ni$(n, \gamma)^{59}$Ni for producing ^{59}Ni, and (3) the daughter nuclide has a half life of 75 thousand years. The cross section of ^{61}Ni$(n, 2p)^{60}$Fe is small (less than 1 mb at 14 MeV) but the product half life is 0.3 million years; the importance of this cross section for fusion reactor design may need to be established.

5. CONCLUSION

The present NEANDC meeting has drawn our attention to review the important activation cross sections included in the preliminary ENDF/B-VI general purpose files and led to plans for remedial work for the neglected ones. It is hoped that the present review of 37 activation cross sections, many of them improved significently over ENDF/B-V, will help data library assemblers in making choices and experimentalists in paying attention to data perceived to be needed from the view point of evaluators.

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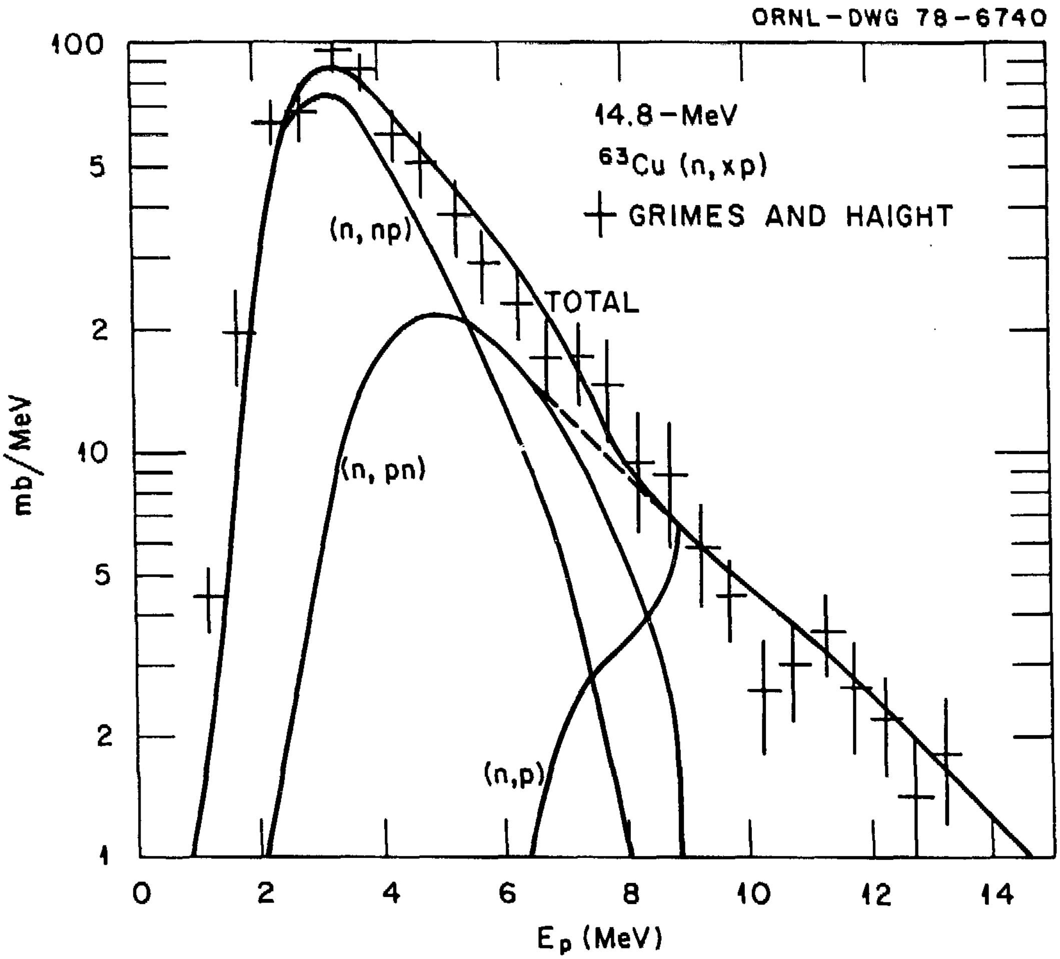

Fig. 1. A model analysis of the measured proton spectrum to extract 14.8-MeV ^{63}Cu(n,p), (n,np), and (n,pn) cross sections. The data are from Grimes and Haight (ref. 14) and the model code used is TNG (ref. 13).

Table 1. Activation Cross Section Summary

Element	Key	Reaction	Half Life
Cr	7	$^{50}Cr(n,\gamma)^{51}Cr$	27.7 d
	3	$^{52}Cr(n,2n)^{51}Cr$	27.7 d
	6	$^{50}Cr(n,np)^{49}V$	330 d
	8	$^{50}Cr(n,d)^{49}V$	330 d
	4	$^{50}Cr(n,2n)^{49}Cr$	42 m
Fe	7	$^{54}Fe(n,\gamma)^{55}Fe$	2.7 y
	3	$^{56}Fe(n,2n)^{55}Fe$	2.7 y
	7	$^{54}Fe(n,\alpha)^{51}Cr$	27.7 d
	1	$^{54}Fe(n,p)^{54}Mn$	313 d
	1	$^{56}Fe(n,p)^{56}Mn$	2.6 h
	6	$^{54}Fe(n,np)^{53}Mn$	3.7×10^6 y
	8	$^{54}Fe(n,d)^{53}Mn$	3.7×10^6 y
	7	$^{58}Fe(n,\gamma)^{59}Fe$	45 d
Ni	1	$^{58}Ni(n,p)^{58}Co$	71 d
	3	$^{58}Ni(n,2n)^{57}Ni$	36 h
	6	$^{58}Ni(n,np)^{57}Co$	271 d
	8	$^{58}Ni(n,d)^{57}Co$	271 d
	3	$^{58}Ni(n,\alpha)^{55}Fe$	2.7 y
	5	$^{60}Ni(n,p)^{60}Co$	5.27 y
	7	$^{62}Ni(n,\gamma)^{63}Ni$	100 y
	2	$^{58}Ni(n,\gamma)^{59}Ni$	7.5×10^4 y
	9	$^{60}Ni(n,2n)^{59}Ni$	7.5×10^4 y
	9	$^{61}Ni(n,2p)^{60}Fe$	3×10^5 y
	6	$^{62}Ni(n,\alpha)^{59}Fe$	45 d
Cu	7	$^{63}Cu(n,\gamma)^{64}Cu$	12.7 h
	1	$^{65}Cu(n,2n)^{64}Cu$	12.7 h
	1	$^{63}Cu(n,2n)^{62}Cu$	9.74 m
	3	$^{63}Cu(n,p)^{63}Ni$	100 y
	8	$^{65}Cu(n,t)^{63}Ni$	100 y
	1	$^{63}Cu(n,\alpha)^{60}Co$	5.27 y
Pb	3	$^{204}Pb(n,2n)^{203}Pb$	52 h
	8	$^{204}Pb(n,p)^{204}Tl$	3.8 y
	9	$^{206}Pb(n,nd)^{204}Tl$	3.8 y
	8	$^{206}Pb(n,t)^{204}Tl$	3.8 y
	7	$^{204}Pb(n,\gamma)^{205}Pb$	1.4×10^7 y
	3	$^{206}Pb(n,2n)^{205}Pb$	1.4×10^7 y
	8	$^{206}Pb(n,\alpha)^{203}Hg$	46.8 d

Key: 1 – Sufficient data, GLUCS analysis
2 – Sufficient data, SAMMY analysis
3 – Sufficient data, TNG calculation
4 – Curve drawn through data
5 – Conflicting data, integral data used
6 – Insufficient data, TNG calculation
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