International Conference on Nuclear Data for Science and Technology 2007
DOI: 10.1051/ndata:07362

Evaluations of the fast neutron cross sections of ^{182,183,184,186}W and ^{181}Ta including complete covariance information

S. Tagesen[1], H. Vonach[1], and A. Wallner[1]

[1]Isotope Research and Nuclear Physics, Faculty of Physics, University of Vienna, 1090 Vienna, Austria

Abstract. New evaluations of all important neutron cross sections of ^{182,183,184,186}W and ^{181}Ta were performed from the upper end of the resonance region (2.2–12 keV) up to 20 MeV. The evaluation combines the results of recent nuclear model calculations (prior) and the complete existing experimental data base by means of the Bayesian code GLUCS06 in order to obtain the most accurate description of the cross section (posterior) within our present knowledge. As result of this work we obtained improved file 3 (cross sections) and file 33 (covariances) data for all important reactions of fast neutrons with the mentioned nuclides. Whenever necessary and possible fine structure of cross sections (at low neutron energies) was superimposed on the GLUCS results for the cross sections in a final evaluation step. For the isotopes of W complete new evaluated general purpose files in ENDF-format were produced by combining our evaluation results (files 3 and 33) with existing resonance data from JENDL 3.3 and file 4 and 6 data (energy-angle distributions for secondary particles) from our prior. These evaluations have been accepted for the Joint European Fission and Fusion File JEFF-3. For Ta a complete new evaluated file based on the described evaluation of cross sections and covariances will be produced in near future and submitted to JEFF-3.

1 Introduction

Feasibility studies for and implementation of new large scale facilities in the field of nuclear technology, e.g., the fusion reactor ITER, frequently pose reliability requirements which can hardly be fulfilled by currently available nuclear data files. To improve this situation our group at Vienna University has started in 1990 a program to update the data files for several important materials as Fe, Cr, Be and more recently, Ni, Si and Ti. The work is done as part of the EFF working group, which guarantees a rigorous quality assurance procedure by running through a full benchmarking cycle.

2 General evaluation procedure

The general principle of our evaluation is essentially the same as described in ref. [1]. For a better understanding we will give a short description of this procedure; it is shown schematically in figure 1 for ^{184}W. First we choose a set of non-redundant cross sections which give a complete, sufficiently detailed description of the interaction of fast neutrons with the respective nuclide as the subject of the evaluation. As the starting point we use our prior knowledge of the neutron cross sections from nuclear model calculation. Each type of cross section is represented by a cross section vector T and its covariance matrix M. Then Bayes' theorem is used to add successively the experimental data for the various isotopic W cross sections to the prior. This is done in the following way: if the data are described by a vector R with the covariance matrix V, application of Bayes' theorem results in the following relations for the improved cross sections T′ and its covariance matrix M′

$$\mathrm{T}' = \mathrm{T} + \mathrm{MG}^{+}(\mathrm{GMG}^{+} + \mathrm{V})^{-1}(\mathrm{R} - \mathrm{R_T}) \qquad (1)$$

$$\mathrm{M}' = \mathrm{M} - \mathrm{MG}^{+}(\mathrm{GMG}^{+} + \mathrm{V})^{-1}\,\mathrm{GM} \qquad (2)$$

where R_T presents the prior value interpolated at the point where R is given, G is the sensitivity matrix of the new experimental data relative to the prior data with the matrix elements $g_{ij} = dR_i/dT_j$, and the up scripts (+) and (−1) mean transpose and inverse operation respectively.

From this procedure (depicted at the left side of fig. 1) we get a set of improved cross sections with much reduced uncertainties compared to the prior values for those cross sections where accurate measurements are available. This procedure however does not use the complete experimental data base. In addition to cross section measurements for our basic cross sections there exist always additional measurements on so-called redundant cross sections, which are sums or differences of our basic, linearly independent cross sections (see fig. 1 and sect. 6). In order to also use this information in a final evaluation step (see right side of fig. 1) the results of our evaluations for the basic cross sections are used as a new improved prior and the data for the redundant cross sections are added as data for the corresponding sums or differences of basic cross sections in a final evaluation step again using equations (1) and (2).

This leads to a final result of the evaluation in form of a cross section vector T′ containing a complete set of independent cross sections and one large covariance matrix M′ which can be subdivided into covariance matrices for the individual cross sections and covariance matrices between different cross section types (interreaction covariance matrices). Technically this procedure is performed by means of the code GLUCS ref. [2] which implements equations (1) and (2) and provides output on T′ and M′ directly in ENDF/B format.

Recently we have modified the code [3] by using the inverse squares of the relative uncertainties of the experimental cross sections as weights instead of the absolute cross section uncertainties as before. The modification removes a small bias towards too small evaluated cross sections and makes the code much less sensitive to inconsistencies in the experimental data base.

3 Establishment of the prior cross sections and covariances

As necessary for a general purpose evaluation we chose a complete set of non-redundant basic cross sections from which all other cross sections can be calculated as linear functions of these basic cross sections.

For all isotopes this set included the cross section $\sigma_{n,2n}$(MT16), $\sigma_{n,3n}$ (MT17), $\sigma_{n,n\alpha}$(MT22), $\sigma_{n,2n\alpha}$ (MT24), $\sigma_{n,np}$ (MT28), $\sigma_{n,2np}$ (MT41), $\sigma_{n,n\ cont}$ (MT91), $\sigma_{n,\gamma}$ (MT102), $\sigma_{n,p}$ (MT103), $\sigma_{n,d}$ (MT104), $\sigma_{n,t}$ (MT105), $\sigma_{n,3He}$ (MT106), and $\sigma_{n,g\alpha}$(MT107).

Slightly different choices were made for inelastic scattering with excitation of discrete levels for the different isotopes. For all isotopes we chose a total number of 5 groups for the description of inelastic scattering to the discrete low-lying levels. These groups were:

^{182}W: (n,n1), (n,n2), (n,n3), (n,n4–10), and (n,n11–19)

^{183}W: (n,n1), (n,n2), (n,n3–4), (n,n5–8), and (n,n9–14)

^{184}W: (n,n1), (n,n2), (n,n3), (n,n4–10), and (n,n11–18)

^{186}W: (n,n1), (n,n2), (n,n3), (n,n4–10), and (n,n11–18)

^{181}Ta: (n,n1), (n,n2–3), (n,n4–5), (n,n6–10), and (n,n11–20).

This lumping of levels of course involves only the evaluation process. In the final file 3 the individual levels will again be separate, however covariances (file 33) will be available only for the described level groups. It was agreed within the JEFF community, that our evaluation should be identical with the Pereslavtsev evaluation apart from the adjustment of the cross sections to the experimental data base. Accordingly Pereslavtsev cross sections refs. [4,5] were used as prior cross sections for all our evaluations, except for a few rare reactions which had not been calculated by Pereslavtsev.

Covariances for the used prior cross sections were estimated for all prior cross sections in the following way:

1. Uncertainties:
   All prior cross sections were compared to the results of recent TALYS calculations and the cross sections from JENDL 3.2 (mostly derived from GNASH' calculations) and uncertainties were estimated from the discrepancies between these 3 sets of excitation functions. For a number of rare reactions, with very small cross sections, which are very uncertain, we assumed an uncertainty of ±90%, which is about the largest uncertainty, which can be reasonably handled within the ENDF/BVI covariance formalism.
2. Correlations:
   For all prior cross sections a triangular decrease of correlation with increasing distance in energy was assumed in order to describe the (positive) correlations between the cross section uncertainties at different neutron energies E_1 and E_2 as described in ref. [1].

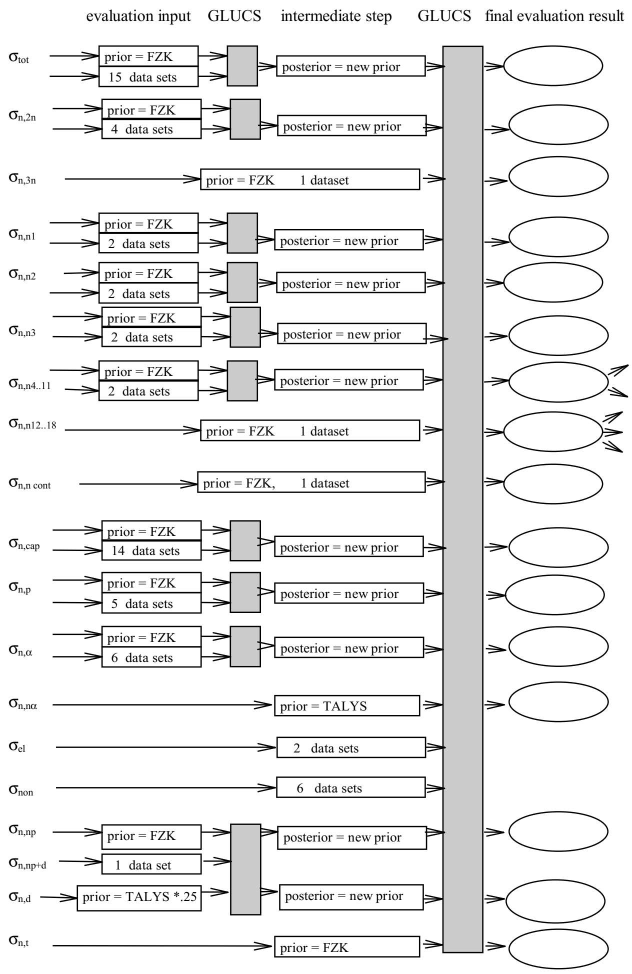

Fig. 1. ^{184}W evaluation flow chart.

4 Establishment of the experimental data base

For the cross section we used the experimental data compiled in EXFOR and CINDA and supplemented them by very recent ones which were mostly obtained directly from the authors. All data sets were critically reviewed. Measurements which were obviously incorrect or of negligible impact to the evaluation were rejected.

We assumed that the covariance matrix of total uncertainties can be split into two matrices of partial uncertainties:

– a diagonal covariance matrix of partial uncertainties describing short-energy-range (SER) correlation properties such as statistical uncertainties due to a finite number of counts per channel;
– a constant covariance matrix of partial uncertainties connected with properties which induce large-energy-range (LER) correlations, such as systematic uncertainties due to any normalization of the cross sections in order to get absolute values, to the determination of the number of nuclei in a sample, to geometrical sizes and distances and to sample self-absorption properties for the non resonance energy region. This means we assume complete correlation over all energy groups for these long range uncertainty components.

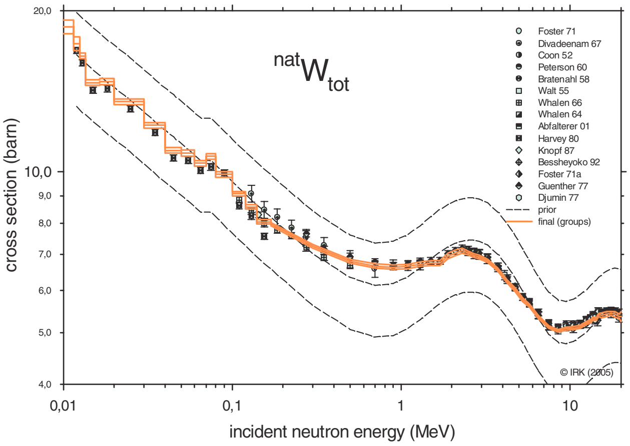

Fig. 2. Evaluated group cross sections for σ_{tot} for ^{nat}W.

The magnitudes of the described two components were chosen according to the uncertainty information given by the authors, or in case of missing information they were estimated by the evaluators according to their experience about typical uncertainties at the time of the respective experiments.

5 Calculation of the evaluated cross sections and covariance

In a first evaluation step, priors for the cross section and experimental data were combined separately for each reaction channel (left side of fig. 1) for all cases where experimental data exist. For the second step (right side of fig. 1), all cross sections for all energies are combined into one large cross section vector with one covariance matrix consisting of the covariance matrices for all reactions and zero inter-reaction covariance matrices. This joint cross section vector was combined with the redundant cross sections (σ_{el}, σ_{non} and σ_{inel}) in a final application of equations (1) and (2). The cross sections σ_{non} and σ_{el} are expressed for this purpose in terms of basic cross sections in the following way

$$\sigma_{\rm non} = \text{sum of all basic cross sections except } \sigma_{\rm tot} \quad (3)$$

$$\sigma_{\rm el} = \sigma_{\rm tot} - \sigma_{\rm el} \quad (4)$$

$$\sigma_{\rm inel} = \sigma_{\rm n,n\ cont} + \Sigma\sigma_{\rm n,ni}. \quad (5)$$

Because of the conditions equations (3–5) and the consideration of all basic cross sections as one coupled set, the resulting correlation matrix now includes parts, which describe correlations between different energy intervals of different cross sections. In most cases these correlations are small (<10%), in some cases however, e.g., between different partial **i**nelastic cross sections, they are important and have to be taken into account.

Finally (as also indicated in fig. 1) the lumped cross sections for discrete inelastic scattering to groups of level was split in cross sections for inelastic scattering for each level, by splitting the group cross sections in proportion to the cross section ratio in the prior cross sections.

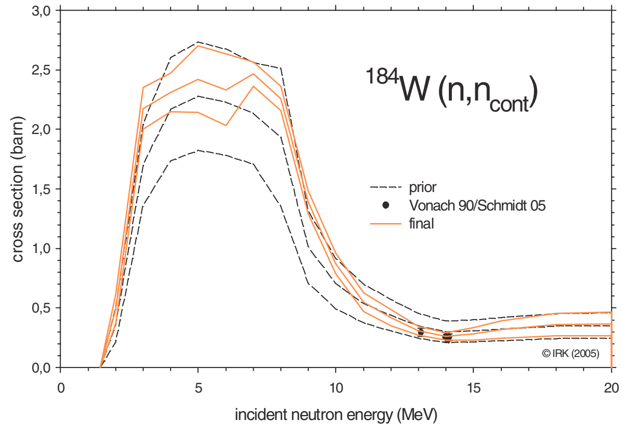

Fig. 3. Evaluation results and experimental data base for $\sigma_{n,ncont}$ for ^{184}W.

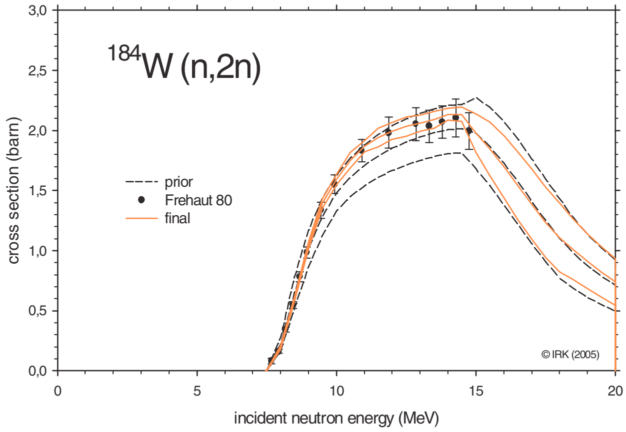

Fig. 4. Evaluation results and experimental data base for $\sigma_{n,2n}$ for ^{184}W.

6 Results of the evaluation

The main result of this evaluation is a complete but non-redundant set of cross sections and their covariances in the fast neutron energy range 12 keV–20 MeV for ^{182,184,186}W, 2.2 keV–20 MeV for ^{183}W and 2.4 keV–20 MeV for ^{181}Ta for the cross sections listed in section 3. For all W-isotopes the evaluated total cross sections for ^{nat}W is used for the reasons outlined in ref. [1].

As an example for the evaluation results the evaluated cross section, their uncertainties and the accepted experimental data are shown for σ_{tot} for ^{nat}W (used for all W-isotopes) and $\sigma_{n,\gamma}$, $\sigma_{n,ncont}$ and $\sigma_{n,2n}$ for ^{184}W in figures 2–5.

Results for the rest of the nuclides are similar. As the figures show rather small uncertainties could be obtained, which will allow satisfactory neutron transport calculations in most cases.

7 Construction of the complete evaluated files for ^{182,183,184,186}W

As already discussed our evaluations were done with the intent to be as much as possible compatible with the recent

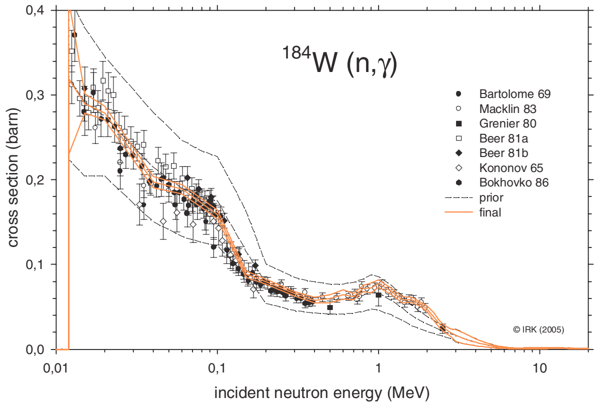

Fig. 5. Evaluation results and experimental data base for $\sigma_{n,\gamma}$for ^{184}W.

evaluations of Pereslavtsev et al. ref. [4]. Accordingly our evaluations were produced as modifications of the Pereslavtsev evaluations.

In detail the following changes to these evaluations were made:

File 1 was amended by a description of the changes performed in this work.

In file 2 the resonance parameters from ENDF/BVI.8 used by Pereslavtsev for W were replaced by the more recent resonance parameters of JENDL 3.2, which extend to considerably higher energies.

File 3. All cross sections above the resonance region were replaced by results of this work. Total cross sections (MT1) for W contain the measured fine structure from Harvey 80 ref. [6] for energies below 170 keV. All other cross sections are the direct results of our GLUCS evaluation.

File 4–15 of the Pereslavtsev evaluation remained unchanged. File 33 (Covariance data) was added for all cross sections in file 3 for the whole energy range above the resonance region (that is above 12 keV for ^{182,184,186}W, above 2.2 keV for ^{183}W, and above 2.4 keV for ^{181}Ta). In addition approximate covariances for MT1 (σ_{tot}) and MT102 ($\sigma_{n,\gamma}$) for the thermal and resonance region are also given in a two group structure as MF33 data.

The evaluations for ^{182,183,184,186}W have been accepted for the JEFF-3 library (Joint European Fission and Fusion File), the ^{181}Ta evaluation has recently been submitted to JEFF.

References

1. H. Vonach, S. Tagesen, *Proc. Int. Conf. on Nuclear Data for Science and Technology*, *Santa Fe, 26 Sept.–1 Oct. 2004* (Melville, NY, 2005), p. 308.
2. S. Tagesen, D.M. Hetrick, *Proc. Int. Conf. on Nuclear Data for Science and Technology*, *Gatlinburg, May 1994*, Vol. 1 (ANS, 1994), p. 589.
3. S. Tagesen, H. Vonach, EFF-Doc 878 (2003).
4. P. Pereslavtsev, U. Fischer, *Proc. Int. Conf. on Nuclear Data for Science and Technology*, *Santa Fe, 26 Sept.–1 Oct. 2004* (Melville, NY, 2005), p. 215.
5. P. Pereslavtsev, U. Fischer, Nucl. Instrum. Meth. **248**, 225 (2006).
6. J.A. Harvey (private communication).