Turk J Phys
31 (2007) , 109 – 116.

Evaluations of Resonance Parameters and Resonance Integral of Tungsten

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Received 08.11.2005

Abstract

I present evaluated values of resonance parameters and resonance integral for natural tungsten on the basis of experimental transmissions data obtained at the Pohang Neutron Facility (PNF), Republic of Korea. Resonance parameters were obtained by using the Bayesian code SAMMY. The output values of SAMMY were used to evaluate the resonance integral for the capture cross-section.

Key Words: linear accelerator, transmissions, cross-sections, resonance parameters, resonance integral, SAMMY code

1. Introduction

High-resolution neutron transmission experiments in time of flight (TOF) method with pulsed electron linear accelerators (e-LINAC) are used for the measurement of total cross sections of nuclides in the resolved and un-resolved resonance region. Resonance analysis of the transmission data is done with Oak Ridge National Laboratory (ORNL) shape fitting R-matrix code known as SAMMY [1]. The software package fits a shape to experimental data to determine resonance parameters by solving Bayes' equation. To see the quality of the fit in this fitting procedure, I used the RSAP, a computer code for display of neutron cross section data [2].

Resonance analysis is an important activity in data evaluation. It is known that representation of low energy cross-sections by appropriate resonance formalism permits the simultaneous analysis of several partial and total cross-section measurements done at different temperatures under different energy resolution. The use of a unitary formalism such as the Reich-Moore (RM) formalism ensures consistency in the line shapes of partial and total cross-sections. Several formalisms, viz. Single Level Breit-Wigner (SLBW), Multi Level Breit-Wigner (MLBW) and Adler-Adler (AA), were developed and incorporated in the evaluated nuclear data files. In the recent evaluated nuclear data files, viz. ENDF/B-VI.8, JENDL-3.3, JEF-3.0, BROND-2.2 and CENDL-2, RM formalism is used for all the important nuclides. The main reasons [3] for the use of RM formalism are: (a) the unitary condition is satisfied and (b) it can represent cross sections even when there are multilevel interferences. Hence, in the SAMMY, it is recommend using RM formalism for the data fitting, even though it has options for SLBW and MLBW formalisms.

In this paper I report the resonance parameters of W isotopes by using the n_TOF experimental data of PNF and SAMMY code for the neutron energy up to 100 eV. I have also estimated the capture resonance integrals (RI) to verify the acceptability of the fitted resonance parameters. The uncertainties on the RI due to uncertainties of resonance parameters are also estimated.

2. Collection of n_TOF Spectra

The details experimental arrangement and explanations for the transmission measurements can be found in references [4], [5]. The Pohang Neutron Facility consists of a 100 MeV linear accelerator with a water cooled Ta target, surrounded by the water moderator and around 11 m TOF path length. To reduce the gamma-flash generated by the electron burst in the target, the target is placed in 55 mm away from the center of neutron guide. The target was composed of ten Ta plates of diameter 4.9 cm and effective thickness of 7.4 cm. There was a 0.15 cm water gap between Ta plates in order to cool the target effectively. The target housing was made of titanium. This target was set at the center of a cylindrical water moderator contained in an aluminum cylinder with a thickness of 0.5 cm, a diameter of 30 cm and a height of 30 cm. The water level in the moderator was 3 cm above the target surface. The neutron guide tubes were constructed by stainless steel with two different diameters, 15 cm and 20 cm, and were placed perpendicularly to the electron beam. The neutron collimation system was mainly composed of H_3BO_3, Pb, and Fe collimators, which were symmetrically tapered from a 10 cm diameter at the beginning to a 5 cm diameter in the middle position where the sample changer was located, to an 8 cm diameter at the end of the guide tube where the neutron detector was placed. There was 1.8 m thick concrete between the target and the detector room.

The transmission sample was natural W metal plate of dimensions 10 cm $\times$ 10 cm with 0.2 mm thickness. The purity of the sample was better than 99.9%. A set of notch filters of Co, In, and Cd plates with 0.5 mm, 0.2 mm and 0.5 mm in thickness respectively, was also used for the background measurement. The sample was placed at the midpoint of the flight path and was cycled into the neutron beam by using an automatic sample rotator. The positions of the sample and free positions were chosen in the following sequence: W-open-W-open. The exposure time for the sample position was 15 minutes; for open position, it was also 15 minutes. The total measurements time for this W sample was 50.8 hrs.

During the experiment, the e-LINAC was operated with a repetition rate of 10 Hz, a pulse width of 1.0 μs, and the electron energy of 65 MeV.

The net n_TOF spectra for the sample in and for the open beam are shown in Figure 1, together with the estimated background level obtained by normalized with the notch filters black resonance's fittings.

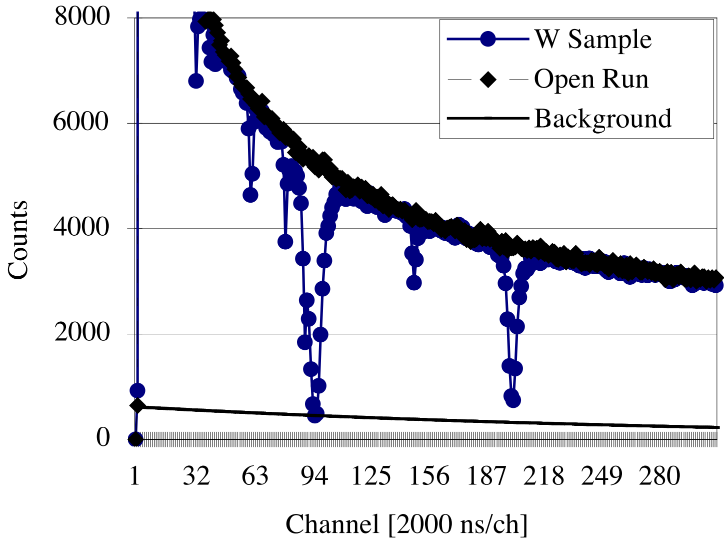

Figure 1. TOF spectra of Tungsten and open run with background level.

The neutron energy E in eV corresponding to each channel I in the TOF spectrum is derived from the relation

$$E = \left\{ \frac{72.3L}{IW - \tau_\circ} \right\}^2 , \tag{1}$$

where L is the neutron flight path in meters, W is the channel width in microseconds and $\tau_\circ$ is the time difference between the start time from the RF trigger and the real time zero when the neutron burst was produced. In this analysis, I used $W = 2.0\ \mu$s (channel width of the CAMAC based DAQ system) and $L = 10.84 \pm 0.02$ m and $\tau_\circ = 2.30 \pm 0.01\ \mu$s.

3. Evaluation of Resonance Parameters

In order to determine the resonance parameters of each resonance peak, I fitted the transmissions as well as total cross-sections data of W with the SAMMY code [1]. The neutron total cross-section can be related to the neutron transmission rate $T(E)$ as follows:

$$\sigma(E) = -\frac{1}{n} \ln T(E); \tag{2}$$

$$T(E) = \frac{[SC - BG]}{[OC - BG]}, \tag{3}$$

where $n$is the samples thickness in atoms/barn; SC, OC and BG are neutron counts for the W, open run, and background measurements, respectively. Equations (2) and (3) are only for the experimental effective values. But in order to estimate the theoretical transmissions as well as cross-sections values depending on the PNF experimental exact conditions I used within SAMMY multilevel R-matrix theory [6] in the Reich-Moore approximation [7] using the following expression for cross-section:

$$\sigma_T = \frac{2\pi}{k^2} g \left\{ 1 - \cos 2\phi \left(1 - \frac{\Gamma_1 \Gamma}{2d} \right) - \sin 2\phi \frac{\Gamma_1 (E_\lambda - E)}{d} \right\}. \tag{4}$$

Here, k is the wave number associated with the incident channel, ϕ the potential scattering phase shift, g is the spin statistical factor, E is the neutron energy and E_λ is the resonance energy. Γ and Γ_1 are the sum of partial widths and a partial width of decay channel 1, respectively. Factor d can be defined as

$$d = \left\{ (E_\lambda - E)^2 + \left(\frac{\Gamma}{2} \right)^2 \right\}. \tag{5}$$

In the SAMMY code Bayes' theorem (generalized least squares) is used to fit the transmissions data to get the resonance parameters of the target sample. For Doppler broadening and resolution analysis, the MULTI method [8] is applied; the free gas model is applied to the Doppler broadening and the convolution of Gaussian and exponential function to the resolution. Resolution function $R(E, E')$ used in this evaluation and its mathematical expression is

$$R_{GE}(E, E') = \frac{1}{\Delta_E \Delta_G \sqrt{\pi}} \int_{E - \Delta E_S}^{\infty} dE^0 \exp\left\{ -\frac{\left(E^0 - (E - \Delta E_S)\right)}{\Delta_E} \right\} \exp\left\{ -\frac{\left(E' - E^0\right)^2}{\Delta_G^2} \right\}, \tag{6}$$

where the width of Gaussian resolution function Δ_G is given by

$$\Delta_G = E\left[aE + b\right]^{1/2} \tag{7}$$

and the width of exponential resolution function Δ_E is given by

$$\Delta_E = cE^{3/2}. \tag{8}$$

The energy shift ΔE_S, which is automatically determined in the SAMMY, is introduced in order to locate the maximum of the broadening function at$E' = E$. Considering the experimental condition observed in the W analysis, as explained in the section 2, the values of constants a, b, and c are computed to be 1.36 $\times 10^{-6}$ eV^{-1}, 9.13 $\times 10^{-6}$, and 6.40 $\times 10^{-4}$ eV$^{-1/2}$, respectively.

Though I analyzed a natural tungsten metallic sample, in reality natural tungsten consists of seven isotopes, four considered the dominant fractions [9]: 26.56% ^{182}W, 14.28% ^{183}W, 30.64% ^{184}W, and 28.43 ^{186}W. I fitted the transmissions data of the natural W sample via the SAMMY code to evaluate the resonance parameters of each resonance peak of the mentioned major four dominated abundances W isotopes in the neutron energy up to 100 eV. Thus the resonance parameters, listed in Table, have been obtained from the resonance shape in transmission data and are compared with those of Mughabghab [9] and ENDF/B-VI.8 [10]. In the table the quantities J, E, Γ_γ, and Γ_n are the spin of a particular resonance, the resonance energy, the gamma width, and the neutron width, respectively. In Figure 2, the experimental transmissions ratios were compared with the SAMMY evaluated results.

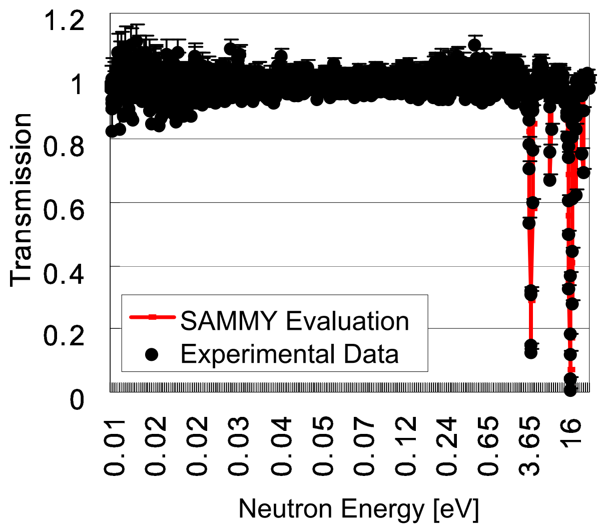

Figure 2. Experimental Transmissions of tunsten with evaluation via SAMMY.

4. Resonance Integral

In nuclear data evaluation, the resonance integral (RI) has an important role to verify the acceptability of the fitted resonance parameters. RI is an independent of resolution and Doppler broadening effects. It is defined as

$$I_\gamma = \int_{E_1}^{E_2} \frac{\sigma_{n,\gamma}(E)}{E} dE , \tag{9}$$

where E_1 and E_2 are the lower and upper energy limits of the integration. It represents the integral of the neutron capture cross sections weighted with a slowing down spectrum $(1/E)$ in the resonance region. The self-shielding effects are not considered in the above definition. If the resonance parameters are available for the SLBW formalism, it can be easily estimated via the relationship [9]

$$I_\gamma \; = \frac{\pi}{2}\, 2.60393 \times 10^6 \left(\frac{A+1}{A}\right)^2 \sum_j \frac{\Gamma_{\gamma\, j}\, g_j\, \Gamma_{n\, j}}{E_j^2\, \Gamma_{t\, j}}, \tag{10}$$

Table. Evaluated Resonance parameters of W isotopes up to 100 eV.

Isotopes	**J**	**E [eV]**		**Γ_γ [meV]**	**Γ_n [meV]**
^{182}W	1/2	Present	-99.998 ± 0.165	65.105 ± 7.766	352.81 ± 26.34
		Ref. [9]	-94	<64>	-
		Ref. [10]	-100	63	2360
	1/2	Present	4.145 ± 0.033	91.623 ± 5.780	1.275 ± 0.005
		Ref. [9]	4.155 ± 0.005	48 ± 3	1.47 ± 0.03
		Ref. [10]	4.160	50	1.47
	1/2	Present	21.206 ± 0.005	531.720 ± 7.693	24.914 ± 0.176
		Ref. [9]	21.060 ± 0.030	65 ± 6	39 ± 1
		Ref. [10]	21.1	62	38
^{183}W	0	Present	-1.535 ± 0.002	50.720 ± 2.884	0.047 ± 0.005
		Ref. [9]	-7.5	70	-
		Ref. [10]	-1.5	66	0.060
	1	Present	7.704 ± 0.006	155.90 ± 16.71	1.768 ± 9.115
		Ref. [9]	7.63 ± 0.03	77 ± 3	1.467 ± 0.160
		Ref. [10]	7.65	70	1.75
	1	Present	27.226± 0.017	51.943 ± 19.800	28.522 ± 6.216
		Ref. [9]	27.05 ± 0.03	77 ± 6	42 ± 2
		Ref. [10]	27.13	77	42
	1	Present	46.318 ± 0.035	250.500 ± 5.741	111.460 ± 0.147
		Ref. [9]	46.24 ± 0.07	77 ± 8	140 ± 4
		Ref. [10]	46.08	68.999	154
	0	Present	47.986 ± 0.001	159.430 ± 0.469	218.100 ± 0.284
		Ref. [9]	47.80 ± 0.04	78 ± 10	108 ± 10
		Ref. [10]	47.8	77.999	115
^{184}W	1/2	Present	-11.765 ± 0.001	48.615 ± 0.241	1.3345 ± 0.002
		Ref. [9]	-420	<72>	-
		Ref. [10]	-11.76	68	1.63
^{186}W	1/2	Present	18.809 ± 0.001	28.143 ± 1.812	329.700 ± 0.010
		Ref. [9]	18.83 ± 0.03	43.8 ± 1.4	300 ± 15
		Ref. [10]	18.81	49	280

where A is the nuclear mass, $\Gamma_{t\,j} = \Gamma_{n\,j} + \Gamma_{\gamma\,j}$, the total width for resonance j, $\Gamma_{n\,j}$ and $\Gamma_{\gamma\,j}$ are the neutron and gamma width respectively, E_j is the resonance energy and g_j is the statistical spin factor. Since the transmission data W was fitted in RM formalism, equation (10) could not be used for estimating I_γ. Hence, I use equation (9) for this analysis. To evaluate I_γ, it is required to have capture cross-sections. As the neutron TOF data gives only the total cross-sections, I estimated I_γ via the relationship

$$I^{\gamma}_{SAMMY} = I^{total}_{SAMMY} - I^{el}_{SAMMY} \tag{11}$$

where I^{γ}_{SAMMY}, I^{total}_{SAMMY} and I^{el}_{SAMMY} are, respectively, the RI for capture, total, and elastic cross sections obtained from our fitted data. These are estimated as:

$$I^{total}_{SAMMY} = \int_{E_1}^{E_2} \frac{\sigma^{\,total}_{\,SAMMY}(E)}{E}\, dE \tag{12}$$

$$I^{el}_{SAMMY} = I^{el}_{ENDF/B-VI}\, \frac{I^{total}_{SAMMY}}{I^{total}_{ENDF/B-VI}} \tag{13}$$

$$I^{total}_{ENDF/B-VI} = \int_{E_1}^{E_2} \frac{\sigma^{total}_{ENDF/B-VI}(E)}{E}\, dE \tag{14}$$

$$I^{el}_{ENDF/B-VI} = \int_{E_1}^{E_2} \frac{\sigma^{el}_{ENDF/B-VI}(E)}{E}\, dE \tag{15}$$

In the above equations, $I^{total}_{ENDF/B-VI}$ and $I^{el}_{ENDF/B-VI}$ correspond to the RI of total and elastic cross sections from ENDF/B-VI.8 [10]. D. E. Cullen's pre-processed point cross-sections from PREPRO-2004 [11] are used for this purpose. It is also used for evaluating the resonance integral in the energy region outside the measurement (from 100 eV to 100 keV). The uncertainty in the RI is due to uncertainties in the fitted resonance parameters obtained by the SAMMY. The uncertainty Δ_I in I_γ can be written as [12]:

$$\Delta_I = \left[\left[\frac{\partial I_\gamma}{\partial \Gamma_n}\right]^2 \Delta^2_{\Gamma_n} + \left[\frac{\partial I_\gamma}{\partial \Gamma_\gamma}\right]^2 \Delta^2_{\Gamma_\gamma} \right]^{1/2}, \tag{16}$$

where Δ_{Γ_n} and Δ_{Γ_γ} are associated errors in neutron and capture widths. Here, I am considering the error in I_γ from the resonance parameters of one resonance only. These individual uncertainties from each level are added quadratically to obtain Δ_I. The expression used for estimating the uncertainty Δ_I in the RI is the following:

$$\Delta_I = 2.608 \times 10^6 \left(\frac{A+1}{A}\right) \sum_j g_j \left[\delta I^2_{\gamma\,j} + \delta I^2_{n\,j}\right]^{1/2} \tag{17}$$

$$\delta I^2_{\gamma\,j} = \left\{ \int \frac{\Gamma_{\gamma\,j}\left(\Gamma^2_{\gamma\,j} - \Gamma^2_{n\,j} + 4\,(E - E_{0\,j})^2\right)}{\left[4\,(E - E_{0\,j})^2 + (\Gamma_{n\,j} + \Gamma_{\gamma\,j})^2\right]^2} \frac{1}{\sqrt{E\,|E_{0j}|}} \frac{dE}{E} \right\}^2 \Delta^2_{\Gamma_{\gamma\,j}} \tag{18}$$

$$\delta I_{nj}^2 = \left\{ \int \frac{\Gamma_{nj}\left(\Gamma_{nj}^2 - \Gamma_{\gamma j}^2 + 4\,(E - E_{0j})^2\right)}{\left[4\,(E - E_{0j})^2 + (\Gamma_{nj} + \Gamma_{\gamma j})^2\right]^2} \frac{1}{\sqrt{E\,|E_{0j}|}} \frac{dE}{E} \right\}^2 \Delta_{\Gamma_{nj}}^2 \tag{19}$$

A detailed derivation of the above expression is given in ref. [12].

The computed resonance integral for the capture cross-section for this work is 322 ± 15, Mughabghab [13] value is 352 ± 25, and ENDF/B-VI.8 [10] value is 362 barns. To obtain this ENDF/V-VI.8 value I carried integration on the capture cross-sections data of ENDF/V-VI.8 from 0.5 eV to 100 keV.

5. Conclusions

The experimental transmission data obtained at Pohang Neutron Facility and the evaluated data by the SAMMY codes are in good agreement, with chi-sq/N value of 1.33. In this analysis negative energy resonances were also included to account for bound levels and several additional energy resonances were considered to account for the effect of resonances above the SAMMY fitting range. The resonance parameters obtained by this evaluation are generally in good agreement with other reported values [9], [10]. Generated covariance matrices obtained the uncertainties of the resonance parameters with the SAMMY have been shown within results on the basis of uncertainties of the transmissions ratio. The output values by the SAMMY evaluation were used to compute resonance integral for the capture cross-section between 0.5 eV to 100 keV. For the above SAMMY fitted range, the ENDF/B-VI.8 values were taken for the resonance integral evaluation that has very small effect as the most dominated peaks are situated in the SAMMY analyzed regions.

Acknowledgement

The author would like to express his sincere thanks to the staff of the Pohang Accelerator Laboratory for the excellent operation of an electron linear accelerator and strong support during his staying at PNF. The author is also indebted to the PNF experimental group; in particular, Prof. G. N. Kim and Dr. Y. S. Lee for providing raw data and for many fruitful discussions. The author also expresses his sincere thanks to Dr. K. Devan for his series of discussions on this work.

References

[1] N. M. Larson, *RSICC Peripheral Shielding Routine Collection SAMMY-M2a: A Code System for Multilevel R-Matrix Fits to Neutron Data Using Bayes' Equations* (PSR-158, SAMMY-M2a), Oak Ridge National Laboratory (ORNL), USA, (1999).

[2] R. O. Sayer, *RSAP-Royce's SAMMY plotter*, Version 4, ORNL, (2001).

[3] F. H. Fröehner, *Workshop Computation and Analysis of Nuclear Data Relevant to Nuclear Energy and Safety*, ICTP, Trieste, Italy, Feb 10 - Mar 13, (1992).

[4] A. K. M. M. H. Meaze *et. al.*, *J. Kor. Phys. Soc.*, **46,** (2005), 401.

[5] A. K. M. M. H. Meaze *et. al.*, *Proc. of Workshop on Nucl Data Production and Evaluation*, PAL, Korea, (2004), 4.

[6] A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.,* **30,** (1958), 257.

[7] C. W. Reich and M. S. Moore, *Phys. Rev.,* **111,** (1958), 929.

[8] F. A. George, *MULTI, A FORTRAN Code for Least-Square Shape Fitting of Neutron Cross-Section Data Using the Reich-Moore Multilevel Formalism*, (LA-5473-MS), Los Alamos Scientific Laboratory (1974)

[9] S. F. Mughabghab, *Neutron Cross-Sections*, Vol. **1** (Academic Press, N.Y, 1984).

[10] P. F. Rose, *ENDF-201, ENDF/B-VI Summary Documentation*, Revised Version 8, (2001).

[11] D. E. Cullen, *The ENDF/B-VI Pre Processing Code*, http://www-nds.iaea.org/ndspub/endf/prepro/

[12] M. J. Trbovich, Ph. D. thesis, Department of Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, New York, 2003.

[13] S. F. Mughabghab, *Thermal Neutron Capture Cross Sections, Resonance Integrals, and G-Factors*, INDC (NDS)-440, IAEA, (2003).