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AVERAGE RESONANCE PARAMETERS FOR NB-93 AND NATURAL TUNGSTEN

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An evaluation of average resonance parameters for niobium-93 and for natural tungsten is accomplished by utilizing the resolved resonance information in the ENDF/B files as well as the results of transmission measurements performed in the range 0.465-200keV. The possibility and the problems of the assignment of average resonance parameter sets to the mixtures of isotopes are discussed.

Introduction

Recently, the nuclear data for some structural materials such as niobium and tungsten have gained increasing importance. Neutron data given in the ENDF/B-4 files for these materials are based on measurements performed at least twenty years ago and consist of a set of resolved resonance parameters and a set of average resonance parameters for unresolved resonance series. In this paper a reevaluation of later data sets is presented by making use the resolved sets given in the ENDF/B-4 files and the results of the transmission experiments for 8 groups of the BNAB system (region 0.465-200keV) published in ref.[1]. In the case of Nb-93 our data simply supersede the average parameters given in the file with MAT=1189 of ENDF/B-4 files , however in the case of tungsten an average parameter set defined for a mixture of isotopes is recommended. In the latter case the statistics of the resolved resonance parameters for tungsten isotopes of masses 182, 183, 184, 186 are used as outgoing data (files with MAT=1128, 1129, 1130, 1131 among the ENDF/B-4 files).

Application of ENDF/B data to correct total cross-sections derived from transmission data

If the transmission samples are thick the experimental values of neutron transmission T_{exp}, show up a strong resonance self-shielding effect especially for lower energy groups. This means that the real transmission rate differs from the attenuation calculated by means of the group-averaged cross-section. The logarithm of their ratio can be used as a measure of the shielding effect. The transmission T_c and the infinite diluted total cross-section, σ_c were calculated from the above mentioned ENDF/B data and used to correct measured total cross-sections against the shielding effect. Thus

$$\sigma^i_{exp}=(\ln T^i_c+\sigma_c h-\ln T^i_{exp})/h_i \qquad (1)$$

for the sample with thickness h_i. This means that the corrected experimental cross-section will be a weighted average as

$$\sigma_{exp}=\sum_i w_i^{-2}\sigma^i_{exp} / \sum_i w_i^{-2} \qquad (2)$$

where

$$w_i=\frac{\Delta T^i_{exp}}{T^i_{exp} h_i}$$

ΔT^i_{exp} is the experimental error for transmission. The error of the group averaged total cross-section is

$$\Delta\sigma^{exp}=\sqrt{(\sum w_i^2)}/N^{3/2}$$

where N is the number of samples.

In the unresolved region formula (1) gives a small correction but in the resolved region, i.e. for the lower energy groups, it considerably changes the results - as can be seen from Figs.1 and 2.

Determination of neutron strength function by fitting the group-averaged total cross-sections

From the experimental total cross-section one may get the neutron strength function by fitting them with the Hauser-Feshbach formula as recommended by the procedures in ENDF/B [2] However it should be taken into account that the Hauser-Feshbach cross-section is an average of a group-averaged cross-section which fluctuates because of the finite number of resonances in this group. Its statistical error z_j, for group j, can easily be estimated by means of the statistics of the group-averaged cross-sections calculated from stochastic resonance series generated in group j [3].

Thus the maximum likelihood function te be minimized is

$$L=\sum_{j=1}^{G}\frac{(\sigma^{exp}_j-\sigma^{HF}_j)^2}{\Delta\sigma^{exp2}_j+z^2_j} \qquad (3)$$

where σ^{HF}_j is the total cross-section

calculated from the average resonance parameters by the Hauser-Feshbach theory.

In parallel with the neutron strength function the γ-width should also be changed. Here we fit to the group-averaged (n,γ) cross-sections calculated from the data given in the ENDF/B files. The likelihood function to be minimized is

$$L_\gamma = \sum_{j=1}^{G} \frac{(\sigma_\gamma - \sigma_\gamma^{HF})^2}{z_\gamma^{j2}}$$

where z_γ^j is the estimated fluctuation error for σ_γ.

Average parameters for Nb-93

The resolved resonance parameters and other cross-section data for Nb-93 found in ENDF/B-4 are based on the data published in refs.[4] and [5]. The resolved energy range is extended to 7.5keV. From 7.5keV to 100keV cross-sections are specified by average resonance parameters. Over 100keV cross-sections are given point-wise.

In Table 1 the average resonance parameters from ENDF/B-4 and those originating from the statistics of resolved resonance parameters are given. For these statistics the method recommended by Frohner[6] has been used. The level densities for different J have been calculated by the formula

$$\rho_J = \text{konst} * [\exp\{-\frac{J^2}{2\sigma^2}\} - \exp\{-\frac{(J+1)^2}{2\sigma^2}\}] \quad (4)$$

derived from the Fermi gas model[6]. For niobium σ=3.3 is recommended[8]. By determining the neutron width for different J the recommendation of Gyulassy-Perkins[7] has been taken into account. It is seen from Table 1 that the average level distance increases with J in contrast to the ENDF/B parameters. The latter follow a $\rho_J=(2J+1)\rho_0$ dependence which is a mistake as the spin of Nb-93 is 4.5 and in this case the more correct formula (4) must be used.

The parameters in column (2) have been used for the outgoing data in the fitting procedure which resulted in the parameters given in column (3).

Two parameters - the s- and p-neutron strength functions - were to be fitted. It can be seen that the s-strength function changed only by 14% while the p-strength function became almost twice larger. This in agreement with the fact that the parameters of p- resonances are known to be worse than those for the s ones.

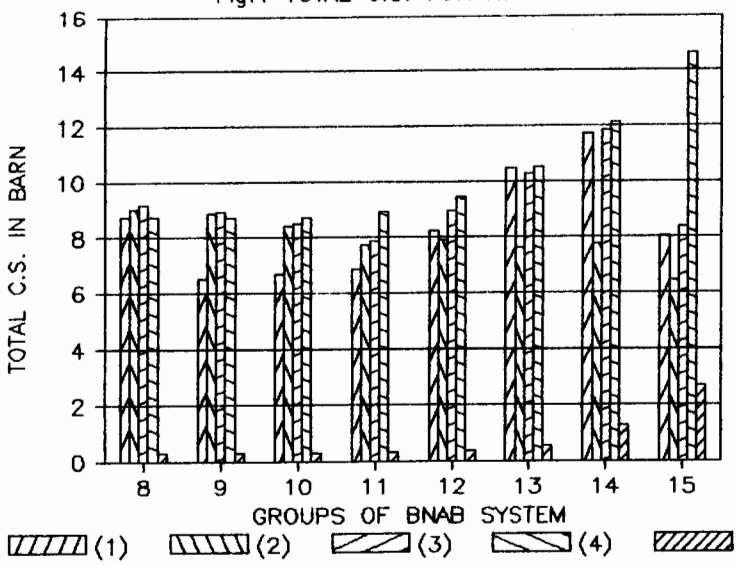
In Fig.1 the group averaged total cross-sections are compared with the uncorrected and corrected experimental total cross-sections (the averaging spectrum is 1/E). It can be seen that the calculation from the original ENDF/B data for the groups in the resolved region (13-15 groups of the BNAB system) agrees well with the corrected experimental results. However, the results of calculation for the groups in the unresolved region (groups 9-11) are essentially lower. The group-averaged total cross-sections calculated from the fitted parameters are represented by the bars (4). The big difference in group 15 relates to a large fluctuation in the distribution of resonances. This is physically acceptable because there are series where the large average distance is accompanied by large average width.

The estimated statistical error for

Table 1 Average parameters for Nb-93

	ℓ=0			ℓ=1		
	(1)	(2)	(3)	(1)	(2)	(3)
S(1)	1.55E-5	4.41E-5	5.00E-5	7.42E-5	2.04E-4	3.98E-4
D(1)	69.795	64.86	64.86	61.19	57.67	57.67
Γ_n(J=3)				1.144E-2	5.37E-2	1.05E-1
D(J=3)				349.6	176.4	176.4
Γ_n(J=4)	1.934E-3	5.08E-3	5.75E-3	1.471E-2	3.01E-2	5.90E-2
D(J=4)	155.1	115.1	115.1	271.9	197.5	197.5
Γ_n(J=5)	2.364E-3	6.55E-3	7.42E-3	1.798E-2	3.88E-2	7.61E-2
D(J=5)	126.9	148.6	148.6	222.5	254.9	254.9
Γ_n(J=6)				2.124E-2	1.14E-1	2.22E-1
D(J=6)				188.3	372.6	372.6
S(J=3)				3.27E-5	3.05E-4	5.96E-4
S(J=4)	1.25E-5	4.41E-5	5.00E-5	5.41E-5	1.52E-4	2.98E-4
S(J=5)	1.86E-5	4.41E-5	5.00E-5	8.08E-4	1.52E-4	2.98E-4
S(J=6)				1.13E-4	3.05E-4	5.96E-4
Γ_γ	2.00E-1	1.923E-1	1.12E-1	2.40E-1	2.074E-1	2.10E-1

Fig.1 TOTAL C.S. FOR Nb-93



(1) calculated from data of file MAT=1189

(2) uncorrected experimental data

(3) corrected experimental data

(4) calculated with fitted parameters

(5) error: $\sqrt{\sigma^{exp2}+z^2}$

the strength of s-resonances is 8.6% and that for the p-resonances is 8.3%. In paper[5] $S_0*10^5=4.\pm0.9$ is given which value agrees well with that given by us. Macklin[9] gives two possible values for S_1*10^4: 2.52±0.29 and a fixed 5.16. Our value - 3.98±0.33 - seems to be in accordance with them. In ref.[10] $S_0*10^5=2.3\pm0.5$ and $S_1*10^4=6.2\pm0.6$ are given, but it is noted by the authors of that paper that S_0 is underestimated because of the strong self-shielding effect.

Average parameters for natural tungsten

It is assumed that the natural tungsten consists of 4 isotopes viz. W-182, W-183, W-184 and W-186 with abundances ρ=0.264, 0.144, 0.306 and 0.284, respectively. In Table 2 the average parameters gained from the statistics of resolved parameters are given. The parameters are only for s-resonances.

In ref.[11] there is an estimation for the strength of p-series: S_1*10^5=7.2, 7.2, 5.8, and 3.7 for the isotopes W-182, W-183, W-184 and W-186, respectively. As the isotopes have nearly equal masses and equal scattering lengths and the single-level Breit-Wigner formalism is applicable to all cases, it seems possible to define average resonance parameters for natural tungsten as a whole.

The formulae underlying the mixture's parameter calculation are

$$D^{J,\ell} = \left(\sum_i \frac{1}{D_i^{J,\ell}}\right)^{-1}$$

for the average distance as follows from a simple physical consideration, and

$$S = \sum \rho_i S_i$$

for the neutron strength function as follows from the fact that the infinite dilute total cross-sections are proportional with the neutron strength function. It is easy to prove that the neutron width gained as a product of the average distance and strength function will satisfy the same statistical law as does that of each component. (It is assumed that the neutron width of each component subjected to the same statistical law.)

As the nuclear spin I is used only for calculating the statistical factor g_j, we may formally introduce one spin for the mixture (in our case I=0) and define J such that we have the same g_J value for resonances from the isotope W-183 whose spin in the ground state is 0.5. In that in the ENDF/B format J is used as the index for unresolved resonance series, we had to introduce formally such compound spins as -0.25 0.25, and 0.75.

Table 2 Average resonance parameters for isotopes of tungsten gained from resolved parameters found in the ENDF/B files

W-182	I=0	J=0.5	D=68.30,	Γ_n=1.91E-2,	S=2.81E-4,	Γ_γ=6.29E-2
W-183	I=0.5	J=0	D=51.71,	Γ_n=1.18E-2,	S=2.28E-4,	Γ_γ=6.75E-2
		J=1	D=18.88,	Γ_n=4.29E-3,	S=2.27E-4,	Γ_γ=6.75E-2
W-184	I=0	J=0.5	D=69.28,	Γ_n=1.98E-2	S=2.86E-4,	Γ_γ=6.87E-2
W-186	I=0	J=0.5	D=79.10	Γ_n=1.84E-2	S=2.33E-4,	Γ_γ=6.45E-2

The parameters in Table 2 were used as outgoing data for fitting in the case of s-resonances. For p-resonances the above mentioned Macklin's values are used to calculate the parameters for different compound series. This calculation is based on the recommendations of paper[7].

Because the fitting procedure led to a parameter set in which $S_1 < 10^{-9}$, the p-resonance series was neglected. In Table 3 the outgoing and the fitted parameters are given.

The measured and calculated group averaged total cross-sections are compared with each other in Fig 2. It is seen that the calculation with the original ENDF/B data, the corrected measured cross-sections, and those calculated with the newly introduced average parameters are in excellent agreement. The uncorrected measured data, as mentioned, differ greatly in the lower energy groups.

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Table 3 Average resonance parameters recommended for natural tungsten

ℓ	0			1				
J	-0.25	0.25	0.5	-0.25	0.25	0.5	0.75	1.5
D	51.71	18.88	23.97	54.00	18.00	23.97	10.80	12.00
Outgoing values								
S_n	3.27E-5	3.27E-5	2.42E-4	1.38E-5	1.38E-5	4.75E-5	1.38E-5	4.75E-5
Γ_n	1.70E-3	6.14E-4	5.80E-3	7.45E-4	2.48E-4	1.14E-3	1.49E-4	5.70E-4
Γ_γ	1.2E-2	1.2E-2	1.2E-2	8.8E-3	8.8E-3	8.8E-3	8.8E-3	8.8E-3
S_0=2.75E-4				S_1=7.84E-5				
Fitted values								
S_n	2.46E-5	2.46E-5	1.81E-4					
Γ_n	1.27E-3	4.62E-4	4.34E-4					
Γ_γ	2.33E-2	2.33E-2	2.33E-2					

$S_0 * 10^4 = 2.06 \pm 0.12$ i.e. the estimated statistical error is 5.5%.

Fig.2 TOTAL C.S. FOR TUNGSTEN