Covariance of resonance parameters ascribed to systematic uncertainties in experiments

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Abstract. In resonance analyses, experimental uncertainties affect the accuracy of resonance parameters. The resonance analysis code REFIT can consider the statistical uncertainty of the experimental data when evaluating the resonance parameter uncertainty. However, since the systematic uncertainties are not independent at each measured energy, they must be treated differently from the statistical uncertainty. In the present study, we developed a new method to incorporate the systematic uncertainty coming from sample thickness into the uncertainty of resonance parameters. We applied this method to transmission of natural zinc measured at ANNRI of MLF in J-PARC and derived the systematic uncertainty of resonance parameters. We found that some of resonance parameters have larger systematic uncertainties than the statistical ones.

1 Introduction

The experimental uncertainties of cross-section measurements in neutron time-of-flight (TOF) method consist of statistical and systematic uncertainties. Furthermore, the systematic uncertainty can be separated into neutron-energy dependent and independent terms. The neutron-energy dependent term contains the uncertainties of, for example, incident-neutron beam spectrum and correction for self-shielding effect, etc. On the other hand, as the neutron energy independent term, the uncertainties of the sample thickness and normalization, etc., can be considered. These independent uncertainties can be represented by only one value and give a uniform relative uncertainty over all energy regions.

Although the resonance analysis code, REFIT [1], can treat the statistical uncertainty, it cannot consider the systematic uncertainty in the resonance analysis. Some methods to treat the systematic uncertainties have been proposed in the literature [2–4]. However, many studies of cross-section measurements have not yet included the systematic uncertainty in their resonance analyses.

We propose a new method to evaluate the systematic uncertainty and correlation of resonance parameters using REFIT. In particular, the uncertainty of sample thickness is discussed because it gives the largest uncertainty in many cases of transmission measurements. In the present work, the resonance analysis of the transmission of natural zinc (Zn) is used as an example.

2 Measurement

The transmission measurement was performed in the Accurate Neutron-Nucleus Reaction measurement Instrument (ANNRI) of the Materials and Life Science Experimental Facility (MLF) in the Japan Proton Accelerator Research Complex (J-PARC). The accelerator in J-PARC with a proton beam power of 700 kW injected two proton pulses (so-called double-bunch mode) with an interpulse of 0.6 μs into the mercury target to generate neutrons. The moderated neutrons were used for the present TOF measurements. A natural Zn sample with the dimensions of 50 × 50 × 6 mm and an areal density of $n_t = 3.92 \pm 0.05$ atoms/barn was used. For the measurements, two different types of Li-glass detectors were employed. A ^{6}Li-enriched glass detector was used to measure transmitted neutrons, whereas a ^{7}Li-enriched glass detector was utilized to estimate the background events due to gamma-rays. The details of transmission measurements are given in Ref [5].

3 Transmission analysis

The transmission analysis was performed in the same manner as described in the past analysis in Ref [5]. Figure 1 shows the pulse height spectrum of the ^{6}Li- and ^{7}Li-glass detectors. The events in the filled color region, where single-hit and double-hit events by ^{6}Li(n,α) reactions were found, were adopted for the present analysis. The dead-time correction was employed using the extended dead-time model [5, 6]. The frame-overlap backgrounds were evaluated by fitting the TOF spectrum between 37 to 40 ms by the following function; $p_1 \exp(-p_2 t) + p_3$. The TOF spectra of two Li-glass detectors after dead-time correction and the estimated frame-overlap spectrum are shown in Fig. 2. To remove gamma-ray backgrounds, the TOF spectrum of the ^{7}Li-glass detector was subtracted from that of the ^{6}Li-glass detector. The TOF spectrum of the ^{7}Li-glass detector was normalized by a factor of 2.2 ± 0.2,

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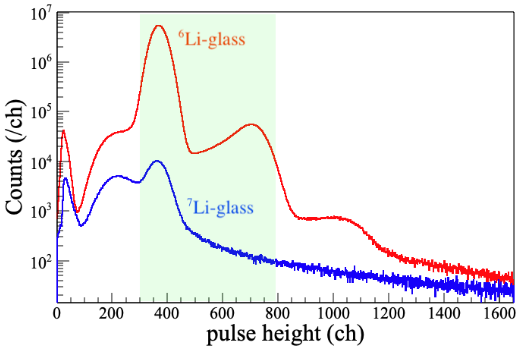

Figure 1. Pulse height spectra of the ^{6}Li- and ^{7}Li-glass detectors. The gated region shown by green is used in the present analysis.

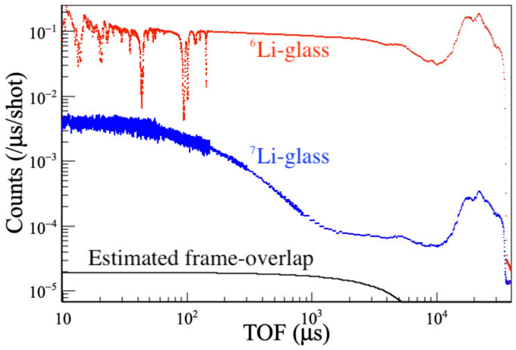

Figure 2. TOF spectra of the ^{6}Li- and ^{7}Li-glass detectors after dead-time correction and estimated frame-overlap backgrounds.

which was derived from the black-resonance in a notch-filter inserted measurement, to correct the difference of the detection efficiencies. The transmission was obtained by dividing the sample-in spectrum from the sample-out spectrum. The obtained transmission is shown in Fig. 3.

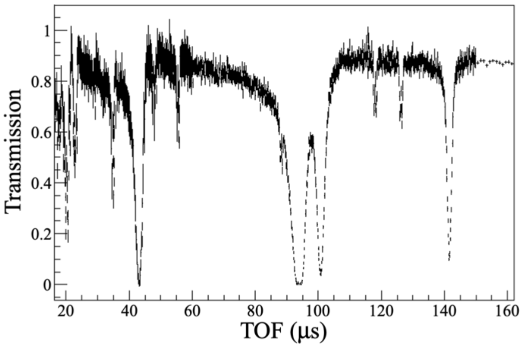

Figure 3. Measured natural Zn transmission.

The reduced total cross section, which includes the resolution function of the MLF and the Doppler broadening, can be calculated by

$$\sigma_{\mathrm{tot}} = -\frac{1}{n_{\mathrm{t}}} \ln T, \tag{1}$$

Table 1. Relative uncertainties of total cross section at two neutron energies.

Neutron Energy [eV]	234	586
TOF [μs]	141	90
Statistical Unc.	3.3%	3.0%
Sample thickness Unc.	1.4%	1.4%
Other systematic Unc.	1.1%	1.2%

where T is transmission. The relative uncertainties of total cross section are listed in Table 1 at two neutron energies. The other systematic uncertainty contains the uncertainties of dead-time correction, beam intensity, and the spectrum normalization factor of the ^{7}Li-glass detector.

4 Resonance analysis and covariance evaluation

The resonance analysis was made using REFIT. As mentioned in Sec. 1, since REFIT does not currently have the ability to evaluate uncertainty of resonance parameters caused by the systematic uncertainty, we derived the sets of resonance parameters with varying sample thickness for the obtained transmission data. The sample thickness of a REFIT input was changed from $n_t - \alpha\Delta n_t$ to $n_t + \alpha\Delta n_t$ dividing into N cases. The systematic uncertainty was calculated as

$$\Delta\Gamma_\eta = \sqrt{\frac{\sum_{i=1}^{N} w_i(\Gamma_{\eta,i} - \overline{\Gamma_\eta})^2}{\sum_{i=1}^{N} w_i}}, \tag{2}$$

where $\Gamma_{\eta,i}$ is the obtained resonance parameter in i-th sample thickness; $\overline{\Gamma_\eta}$ is the obtained resonance parameter for the nominal sample thickness; w_i is the weight calculated by

$$w_i = \frac{1}{\sqrt{2\pi}} \exp(-\beta_i^2), \tag{3}$$

where β_i is calculated by

$$\beta_i = \left(\frac{2(i-1)}{N-1} - 1\right)\alpha, \tag{4}$$

and means that the i-th sample thickness is $n_{\mathrm{t}} + \beta_i \Delta n_t$. The correlation between resonance parameters Γ_η and Γ_ζ was determined as

$$C_{\eta,\zeta} = \frac{\sum_{i=1}^{N} w_i(\Gamma_{\eta,i} - \overline{\Gamma_\eta})(\Gamma_{\zeta,i} - \overline{\Gamma_\zeta})}{\sqrt{\sum_{i=1}^{N} w_i(\Gamma_{\eta,i} - \overline{\Gamma_\eta})^2}\sqrt{\sum_{i=1}^{N} w_i(\Gamma_{\zeta,i} - \overline{\Gamma_\zeta})^2}}. \tag{5}$$

Applying this method, the systematic uncertainty and correlations were estimated. In this estimation, we used $\alpha = 4$ and $N = 9$, i.e. using sample thickness $n_t - 4\Delta n_t$, $n_t - 3\Delta n_t$, $\cdots$, $n_t + 4\Delta n_t$. The neutron width and resonance energy were fitted with fixing the gamma-width to the value in JENDL-5 [7]. Figures 4 and 5 show the fitting result and the definition of resonance number. Because of the double-bunch effect in MLF, some resonances make two dips, such as for resonance No. 6. Resonance No. 11 partially overlapped with resonance No. 12. The obtained correlation of neutron width is shown in Fig. 6. The resulting resonance parameters and uncertainties are listed in Table 2.

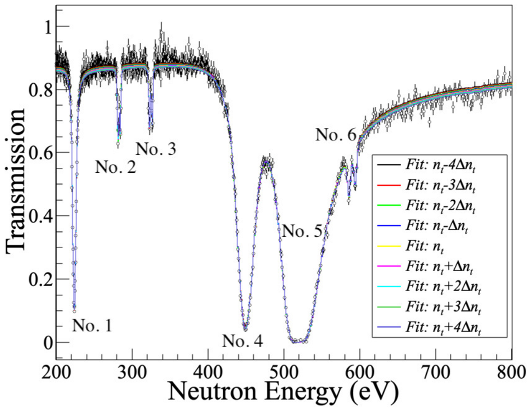

Figure 4. Fitting results for each sample thickness between 200 to 800 eV. The number shows the resonance considered in the present analysis.

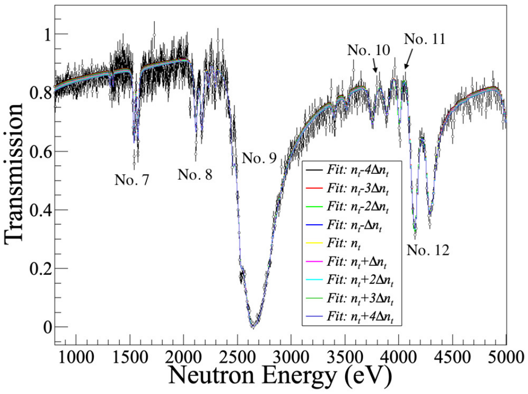

Figure 5. Same as Fig. 4, but in the neutron energy region between 800 to 5000 eV.

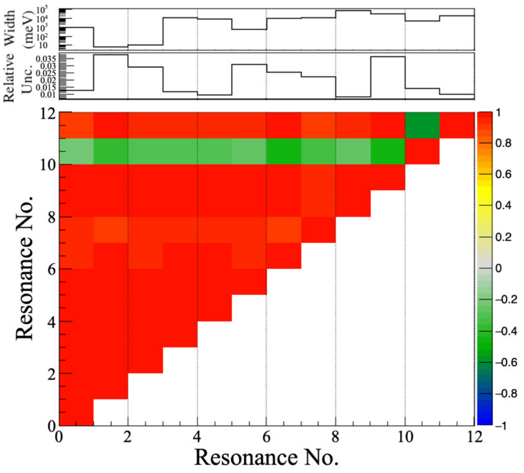

Figure 6. Obtained correlations between neutron widths of all fitted resonances.

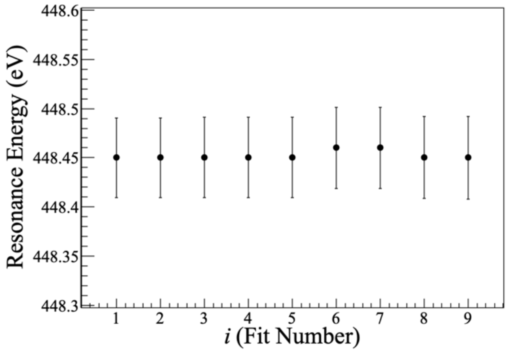

Figure 7. Resonance energy of resonance No. 4 using each sample thickness. The fit number represents which sample thickness was used in fitting such as $n_t - 4\Delta n_t$ for $i = 1$.

5 Discussion

Figure 7 shows the obtained resonance energy of resonance No. 4 for each sample thickness. The error bar represents the fitting uncertainty only considering statistical uncertainty. The resonance energies are consistent regardless of the sample thickness. According to this study, the systematic uncertainty of resonance energy coming from the sample thickness is negligible compared to the statistical uncertainty.

Figure 8 displays the neutron width of resonance No. 4 for each sample thickness. As expected, the neutron width decreases as the sample thickness used in the fitting increases. The systematic uncertainty defined by Eq. (2) corresponds to the slope of this plot. Moreover, the neutron widths for each sample thickness of resonance No. 11 are shown in Fig. 9. In this case, it is difficult to evaluate the systematic uncertainty and correlations among the res-

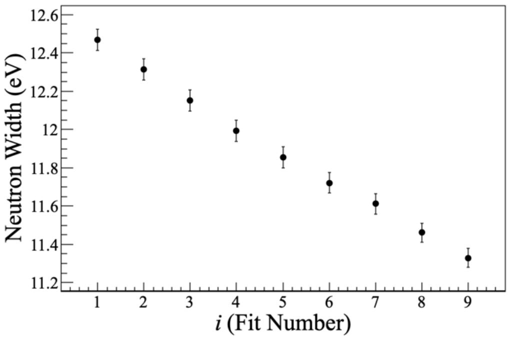

Figure 8. Neutron width of resonance No. 4 for each sample thickness.

Table 2. Obtained resonance parameters. The gamma width was adopted from JENDL-5 [7]. In the neutron width, the first uncertainty represents the fitting uncertainty, and the second uncertainty represents the systematic uncertainty evaluated by Eq. (2). The uncertainty of the resonance energy was deduced from uncertainties of fitting, flight length and initial time delay.

Resonance No.	Reference	Resonance energy (eV)	Neutron width (eV)	Gamma width (eV)
1	Present	223.50 ± 0.02	0.931 ± 0.006 ± 0.012	0.350
	JENDL-5	223	0.771	
2	Present	282.31 ± 0.06	$(6.13 \pm 0.25 \pm 0.23) \times 10^{-3}$	0.294
	JENDL-5	281	0.006	
3	Present	323.84 ± 0.08	$(11.1 \pm 0.7 \pm 0.3) \times 10^{-3}$	0.186
	JENDL-5	323.5	0.011	
4	Present	448.45 ± 0.05	11.86 ± 0.05 ± 0.14	0.650
	JENDL-5	448.2	10.08	
5	Present	517.04 ± 0.07	8.81 ± 0.02 ± 0.08	0.160
	JENDL-5	516.4	8.5	
6	Present	587.95 ± 0.17	0.537 ± 0.034 ± 0.017	0.440
	JENDL-5	587	0.462	
7	Present	1547.7 ± 0.5	8.93 ± 0.33 ± 0.23	0.440
	JENDL-5	1546.2	7.2	
8	Present	2472.2 ± 1.5	12.2 ± 1.7 ± 0.3	0.440
	JENDL-5	2469	10.457	
9	Present	2624.6 ± 0.9	66.2 ± 0.4 ± 0.5	0.500
	JENDL-5	2627	60	
10	Present	3782.5 ± 2.9	31.5 ± 2.6 ± 1.1	0.350
	JENDL-5	3789	31.714	
11	Present	4036.6 ± 1.7	4.60 ± 0.32 ± 0.06	0.198
	JENDL-5	4046	5.2	
12	Present	4165.9 ± 1.3	19.6 ± 0.4 ± 0.2	0.676
	JENDL-5	4170	19.4	

onance parameters since the fitting uncertainty is dominant due to the large statistical fluctuation.

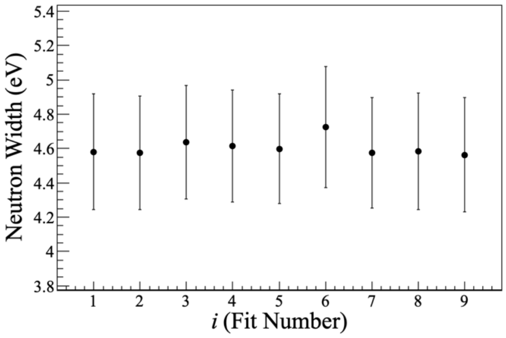

Figure 9. Neutron width of resonance No. 11 for each sample thickness.

If the experimental systematic uncertainty is not considered in the resonance analysis, the total uncertainty of neutron width in some resonances, such as resonances No. 1, 4 and 5, is underestimated. Therefore, it is significant to evaluate the systematic uncertainty in the resonance analyses.

Positive correlations among many resonances were found in Fig. 6. This is an expected result from the following consideration. When the input value of sample thickness in REFIT becomes small, the calculated transmission from a cross-section increases. To reproduce the experimental transmission results, the cross section has to become larger. Therefore, the resonance parameters, especially neutron width, become larger. Such behavior makes the correlation among many resonances positive. On the other hand, a weak negative correlation between resonance No. 11 and the other resonances was found. According to Eq. (5), the correlation with resonance No. 11 should be weak because fitted neutron widths have a flat distribution as seen in Fig. 9. Such "negative" correlation may be incidental.

This technique with reliable resonance parameters is applicable to determining unknown sample thicknesses and sample temperature. The sample thickness can be estimated from the χ^2 distribution by varying an input sample thickness and performing a fit to measured data. Moreover, in the same way as the case of sample thickness, the sample temperature can be deduced by varying an input sample temperature. This way makes use of the resonance broadening due to the Doppler effect as in Kai et al. [8]. The applications to those are underway.

6 Summary

We proposed a new method to derive the systematic uncertainty and correlations among the resonance parameters in the resonance analyses. This is the simple method that the sets of resonance parameters were obtained by changing the input value of the sample thickness in REFIT. The results show that it is essential to consider the systematic uncertainty when deriving the resonance parameters, especially the neutron width, because its contribution to the total uncertainty might be higher than that of the fitting uncertainty.

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