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Determination of the 338 eV, 1098 eV and 1370 eV s-wave resonance parameters for neutron induced reactions of ^{55}Mn at GELINA

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Abstract

In this report new values for the resonance parameters of the 338 eV, 1098 eV and 1370 eV s-wave resonances of ^{55}Mn are presented. The parameters were derived from a resonance shape analysis of transmission and capture data resulting from measurements at the time-of-flight facility GELINA. Special samples have been prepared to optimize the transmission at the resonance dips, to avoid the impact of sample inhomogeneities and to reduce bias effects due to multiple interaction events and the normalization of the capture data. The parameters have been adopted in an ENDF-6 compatible file which has been tested and implemented in the next release of the Joint Evaluated Fission and Fusion data library, *i.e.* JEFF-3.2, which is maintained by the Nuclear Energy Agency of the OECD.

1 Introduction

A validation of the International Reactor Dosimetry File in 2007 by Kodeli *et al.* [1] has pointed out that the cross sections of ^{55}Mn recommended in the major evaluated data libraries cannot predict accurately results of integral benchmarks. The evaluation of resonance parameters for ^{55}Mn performed by Derrien *et al.* [2] has improved significantly the agreement between calculations and results of integral benchmark experiments. This evaluation was strongly based on results of transmission and capture measurements carried out at the time-of-flight facility GELINA of the Institute for Reference Materials and Measurements in Geel, Belgium [3]. Nevertheless, the agreement was not yet satisfactory [4]. The data used in the evaluation of ref. [2] resulted mainly from measurements with powder samples and a relatively thick sputtering target. Since no corrections were applied to account for sample inhomogenities in the powder samples, bias effects for strong resonances are not excluded [5, 6]. In case of the thick sputtering target, the transmission dips of the strong s-wave resonances reach saturation and there is a substantial contribution of multiple interaction events to the capture yield of these resonances [7]. In summary, the experimental conditions of the available data were not ideal to determine the resonance parameters of the strong s-wave resonances at 338 eV, 1098 eV and 1370 eV.

To improve the parameters of these resonances two Mn-Fe alloy samples were prepared and transmission and capture cross section measurements were carried out at GELINA. The advantages of the alloy samples are manifold. Firstly, although the Mn concentration is rather low, its distribution throughout the sample is homogeneous. Inhomogeneities in the ^{55}Mn content that could be introduced, e.g. during the solidification of the alloy, were kept below 0.4%. In addition, the use of an alloy sample containing Fe allows for an internal normalization of capture data using the 1.15 keV resonance of ^{56}Fe and an estimation of the sample induced background due to the neutron sensitivity of the detection system.

2 Experimental conditions

Two Mn-Fe alloy samples were produced. Each disc had a weight of about 32 g, a diameter of 80.1 mm and a thickness of 0.83 mm. The relative amount of ^{55}Mn, in the samples were 5.68 (0.02)at%

Table 1: Characteristics of the samples used for the transmission and capture measurements performed at GELINA. The first column is the reference number. To calculate the areal density the Avogadro constant was taken as $N_A = 6.0221367 \times 10^{23}$ mol^{-1} and the atomic mass for ^{55}Mn as m$_a$ = 54.9380471 u. The uncertainties are standard uncertainties at 1 standard deviation.

Sample ID	**Thickness**	**Area**	**Weight**	**Areal density**	**Mn**
	mm	mm^2	g	at/b $\times 10^{-3}$	at%
TP2010-013-01	0.83	5036.0 (1.0)	32.7685 (0.0008)	7.0215(0.0010)	5.68 (0.02)
TP2010-013-02	0.83	5034.9 (1.0)	32.6678 (0.0003)	7.0078(0.0010)	10.47 (0.04)

Table 2: Relative amount of impurities present in the Fe-Mn alloy samples.

Element	**TP2010-013-01**	**TP2010-013-02**
	wt%	wt%
Al	0.0024	0.0022
Ni	0.0006	0.0007
Cu	0.0011	0.0012
Mo	0.0001	0.00023
C	0.0008	0.0013
S	0.0019	0.0035
O	0.0063	0.0049
N	0.0013	0.0007

and 10.47 (0.04)at%. The elemental composition was determined by inductively coupled plasma mass spectrometry (ICP-MS) and combustion analysis. The distribution of Mn within the samples was verified by X-ray fluorescence. The areal density was based on a measurement of the weight and the area. The latter was determined by an optical surface inspection with a microscope measurement system from Mitutoyo. The characteristics of the samples are given in table 1. The relative amount of impurities are listed in table 2.

The transmission and capture measurements were performed using a moderated neutron beam with the accelerator operating at 800 Hz. The measurement, data reduction and analysis procedures described in ref. [11] were followed. The transmission experiments were carried out at the 50 m station of flight path 4 using a 6.35 mm thick and 101.6 mm diameter NE912 Li-glass scintillator enriched to 95% in ^{6}Li. From the ratio of the sample-in and sample-out spectra, both corrected for dead time and background, the experimental transmission was derived. More details about this measurements station can be found in ref. [8].

The capture experiments were performed at the 60 m capture station of flight path 14. Prompt γ-rays originating from neutron induced capture events were detected by four NE230 cylindrical C_6D_6 liquid scintillators, which were oriented at 125° with respect to the direction of the incoming neutrons. The total energy detection principle in combination with the pulse height weighting technique was applied. The weighting functions were determined by Monte Carlo simualutions as described in ref. [9]. In the calculation of the weighting function the effect of the discrimination level E$_d$ = 150 keV was taken into account. The energy dependence of the neutron flux was measured with a ^{10}B ionisation chamber placed 80 cm before the sample. The ^{10}B chamber was a Frisch gridded ionization chamber with three back-to-back layers of ^{10}B evaporated on a 30-μm-thick aluminium backing, with a total thickness of about 1.25×10^5 at/b ^{10}B and a diameter of 84 mm. From the ratio of the dead time and background corrected weighted response of the C_6D_6 detection system and the neutron flux the experimental yield was derived. The weighted response was only corrected for the time independent background and the time dependent component that does not depend on the sample characteristics. The contribution due to the neutron sensitivity of the detection system was taken into account in the resonance shape analysis. More details about capture cross section measurements at this station can be found in ref. [10].

The AGS code [12], developed at the EC-JRC-IRMM, was used to derive the experimental transmission. The code is based on a compact formalism to propagate all uncertainties starting from uncorrelated uncertainties due to counting statistics. It stores the full covariance information after each operation in a concise, vectorized way. The AGS formalism results in a substantial reduction of data storage volume and provides a convenient structure to verify the various sources of uncertainties through each step of the data reduction process. The concept is recommended by the Nuclear Data Section of the IAEA [13] to prepare the experimental observables, including their full covariance information, for storage into the EXFOR data library [14].

3 Resonance shape analysis

The resonance shape analysis code REFIT [15], based on the Reich-Moore [16] approximation of the R-matrix formalism [17], was used to extract the resonance parameters by adjusting them in a least square fit to the experimental transmissions and capture yields. The code accounts for effects like multiple interaction, neutron sensitivity of the detection system, Doppler broadening and the response of the time-of-flight spectrometer. The version used at the EC-JRC-IRMM includes a module to account for sample inhomogeneities [6] and γ-ray attenuation in the samples. Numerical response functions, which were calculated by Monte Carlo simulations and validated by experiments [18], were used. For the analysis of the transmission data the time response of the detector was introduced by an analytical model included in REFIT.

To account for the the Doppler broadening the free gas model, employing an effective temperature was used. The effective temperature T_{eff} was related to the sample (room) temperature T and the Debye temperature Θ of the sample by [19]:

$$T_{eff} = \frac{3}{8}\Theta \coth\left(\frac{3}{8}\Theta/T\right). \tag{1}$$

According to ref. [20], the Debye temperature for a Fe-Mn alloy is approximately 500K.

The flight path length of the transmission station was adjusted from transmission measurements of ^{238}U, which were analysed with the same response function. The uncertainty of the resulting flight path length L = 47.5865 (0.0040) m is dominated by the uncertainty on the energy of the 6.673 (0.001) eV resonance determined by Derrien *et al.* [21]. The resonance energies and neutron widths were at first adjusted in a fit to the transmission data. The energies of the 338 eV, 1098 eV and 1370 eV resonances derived from the transmission data were used to determine the flight path length L = 58.5714 (0.0050) of the capture station. The uncertainty due to counting statistics was a factor 10 smaller.

The normalization of the capture data was derived from a least squares adjustment in the region of the 1.15 keV resonance of ^{56}Fe with only the normalization factor as an adjustable parameter. The parameters of the 1.15 keV resonance to Γ_n = 61.7 meV and Γ_γ = 574 meV were fixed to the values determined by Perey [22] from transmission measurements at ORELA. This resulted in in a normalization factor N = 0.2114 (0.0024) and 0.2163 (0.0031) for sample TP2010-013-01 and sample TP2010-013-02, respectively. For the final analysis the weighted average N = 0.2136 (0.0030) was used.

For the ^{55}Mn resonances of interest the neutron width is relative large compared to the radiation width. Therefore, the neutron sensitivity of the C_6D_6 detector can introduce a bias on the radiation widths derived from the capture data. Neutron sensitivity of the detector results in a background due to neutrons which are scattered from the sample and create a capture reaction in the sample-detector environment [11]. This background component can be estimated by Monte Carlo simulations or by measuring the response for samples with a high scattering and small capture cross section, such as ^{12}C

Table 3: Resonance parameters (energy E_r, neutron width Γ_γ, radiation width Γ_γ) of the 338 eV, 1098 eV and 2370 eV s-wave resonances of ^{55}Mn. The parameters derived from the experiments described in this work are compared with those recommended in ENDF/B-VII.1. The radiation widths resulting from an analysis without correcting for the neutron sensitivity are also shown.

This work				**ENDF/B-VII.1**		
E$_r$ / eV	Γ_n / eV	Γ_γ / eV		E$_r$ / eV	Γ_n / eV	Γ_γ / eV
		with correction	without correction			
337.63 (0.02)	23.59 (0.03)	0.451 (0.002)	0.453	340.79	23.68	0.410
1097.74 (0.05)	15.92 (0.08)	0.384 (0.003)	0.396	1098.44	15.27	0.397
2370.30 (2.50)	401.00 (5.00)	0.752 (0.020)	0.795	2394.73	403.20	0.783

Table 4: Correlation matrix of the parameters of the 338 eV, 1098 eV and 2370 eV resonance of ^{55}Mn derived from a least squares fit to the transmission and capture data. The parameters of the 338 eV, 1098 eV and 2370 eV resonances are indicated with an upper index (1), (2) and (3), respectively.

	$E_r^{(1)}$	$\Gamma_n^{(1)}$	$\Gamma_\gamma^{(1)}$	$E_r^{(2)}$	$\Gamma_n^{(2)}$	$\Gamma_\gamma^{(2)}$	$E_3^{(3)}$	$\Gamma_n^{(3)}$	$\Gamma_\gamma^{(3)}$
$E_r^{(1)}$	1								
$\Gamma_n^{(1)}$	0.08	1							
$\Gamma_\gamma^{(1)}$	0.01	0.00	1						
$E_r^{(2)}$	0.00	-0.01	-0.02	1					
$\Gamma_n^{(2)}$	0.00	0.00	0.00	-0.06	1				
$\Gamma_\gamma^{(2)}$	0.00	0.00	0.00	-0.01	-0.10	1			
$E_r^{(3)}$	0.00	-0.07	-0.01	0.09	-0.04	0.00	1		
$\Gamma_n^{(3)}$	0.00	-0.10	-0.01	0.11	-0.04	0.00	0.82	1	
$\Gamma_\gamma^{(3)}$	0.00	-0.02	-0.02	0.01	-0.02	-0.03	0.28	0.22	1

and ^{208}Pb. For this work the energy dependence of the neutron sensitivity determined by Borella *et al.* [9, 10] was used in the analysis. The amplitude was adjusted to match the observed yield of the 27.791 keV resonance in ^{56}Fe.

4 Results

The result of a simultaneous least squares adjustment to the transmission and capture data is shown in fig. 1. The experimental transmission and capture yield are compared with the ones calculated with the parameters obtained from the fit and those calculated with the parameters derived by Derrien *et al.* [2], which were adopted in ENDF/B-VII.1 library. The resulting resonance parameters are listed in table 3 and compared with the parameters of ENDF/B-VII.1. The quoted uncertainties are standard uncertainties at one standard deviation which result from only propagating the uncorrelated uncertainties due to counting statistics. The correlation matrix of the fitted parameters is given in table 4. In table 3 the radiation widths resulting from an analysis without accounting for the neutron sensitivity of the detection system are also given. A comparison between the different values for the radiation widths for the 1098 eV and 2370 eV resonance suggests that in the analysis performed by Derrien *et al.* [2] the neutron sensitivity of the detection system was not properly taken into account. The difference in radiation width for the first resonance can be due to a bias in the value of Derrien *et al.* [2] due to the impact of multiple interaction events, as already discussed in ref. [7].

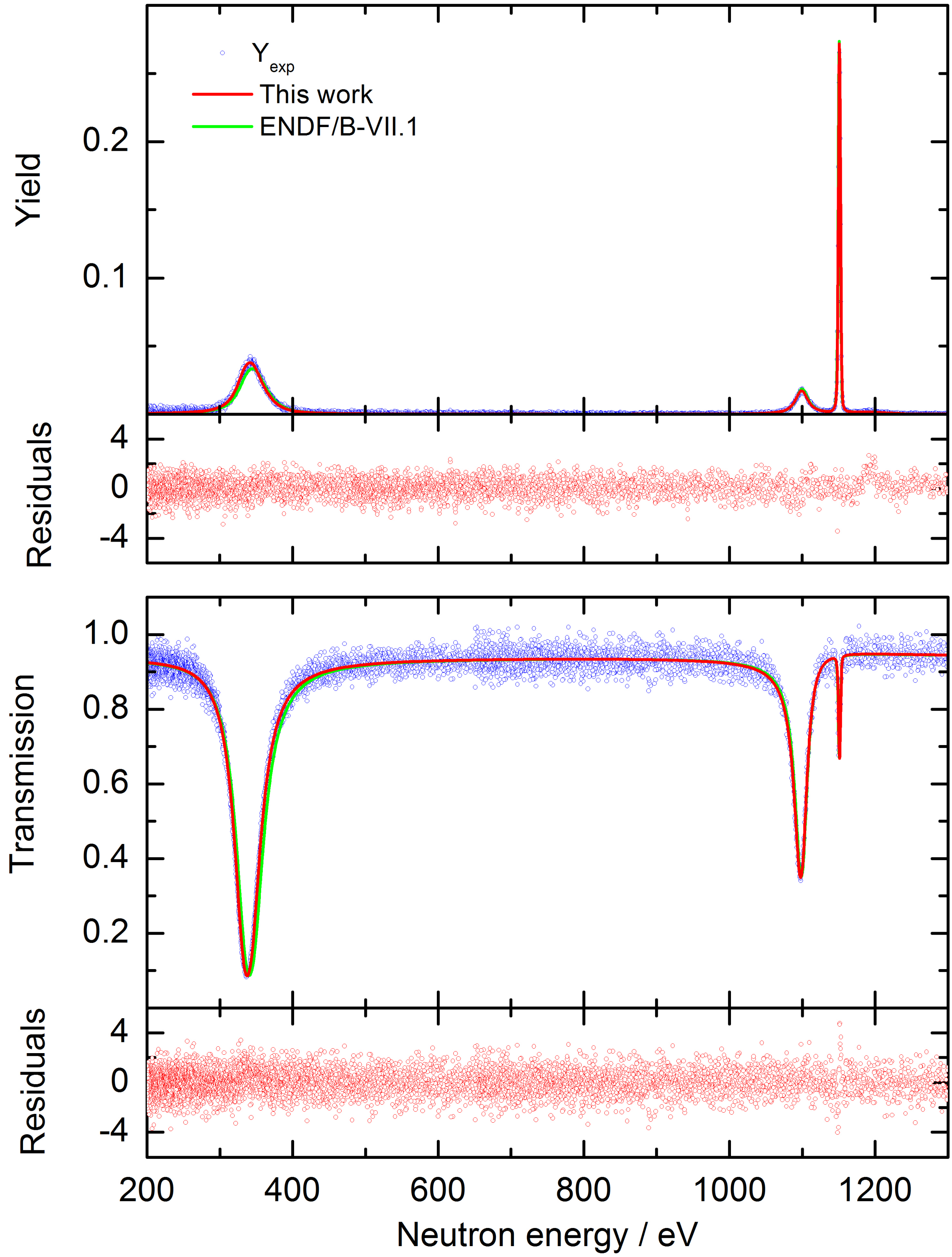

Fig. 1: Experimental capture yield (top) and transmission (bottom) resulting from measurements at GELINA compared to calculations using fitted resonance parameters derived in this work and the ones derived Derrien *et al.* [2] adopted in ENDF/B-VII.1 library. The residuals of the calculations using the fitted resonance parameters are shown for both capture yield and transmission.

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