Neutron resonance parameters of ^{55}Mn from Reich-Moore analysis of recent experimental neutron transmission and capture cross sections

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Abstract

High-resolution neutron capture cross section measurements of ^{55}Mn were recently performed at GELINA by Schillebeeckx et al. (2005) and at ORELA by Guber et al. (2007). The analysis of the experimental data was performed with the computer code SAMMY using the Bayesian approach in the resonance parameters representation of the cross sections. The neutron transmission data taken in 1988 by Harvey et al. (2007) and not analyzed before were added to the SAMMY experimental data base. More than 95% of the s-wave resonances and more than 85% of the p-wave resonances were identified in the energy range up to 125 keV, leading to the neutron strength functions $S_0 = (3.90 \pm 0.78) \times 10^{-4}$ and $S_1 = (0.45 \pm 0.08) \times 10^{-4}$. About 25% of the d-wave resonances were identified with a possible strength function of $S_2 = 1.0 \times 10^{-4}$. The capture cross section calculated at 0.0253 eV is 13.27 b, and the capture resonance integral is 13.52 ± 0.30 b. In the energy range 15 to 120 keV, the average capture cross section is 12% lower than Lerigoleur value and 25% smaller than Macklin value. GELINA and ORELA experimental capture cross sections show a background cross section not described by the Reich-Moore resonance parameters. Part of this background could be due to a direct capture component and/or to the missing d-wave resonances. The uncertainty of 10% on the average capture cross section above 20 keV is mainly due to the inaccuracy in the calculation of the background components.

1. Introduction

Accurate neutron capture cross sections of ^{55}Mn are important for reactor designs in view of its use as alloy structural material. Manganese-55 is also a constituent of structural materials present in fissile material operations, and accurate cross-section data are needed to support criticality safety analyses. The resonance parameters of the most recent evaluated data files are mainly based on the work by Garg et al. (1978) and by Macklin (1985). The work by Macklin was aimed to meet the "World Request of Nuclear Data" (WRENDA 1983/1984) of 10% accuracy in the lowest energy resonances and 20% accuracy up to 100 keV (IAEA, 1983). Recently Perrot et al. (2003) using a lead slowing-down-spectrometer and simulation have shown that the ^{55}Mn-evaluated capture cross sections are inadequate in the energy range of 50 eV to 30 keV. They suggested that re-

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measurement and re-evaluation be performed below the fast energy range.

The aim of the present work was to perform a SAMMY Reich-Moore analysis of recent experimental ^{55}Mn neutron transmission and capture data in an attempt to obtain more accurate resonance parameters in the thermal energy range to 125 keV, below the first inelastic channel.

2. The experimental data base and the conditions of the analysis

The experimental data base includes the 1988 neutron transmission of Harvey et al. (2007), the 2005 GELINA capture cross section measurement of Shillebeeckx et al. (2007) and the 2007 ORELA capture measurement of Guber. (2007). The experimental resolution of the capture data allowed a good separation of the resonances up to about 120 keV neutron energy. For the evaluation of the cross sections in the thermal energy range, earlier measurements were added to the experiment data base: total cross section from Cote et al. (1964) and Rainwater et al. (1947) and capture cross section from Widder et al. (1975). The sample used in GELINA and ORELA capture measurements had thicknesses of 0.0190 at/b and 0.0178 at/b, respectively, resulting in large self-shielding and multiple scattering effects. The updated version of SAMMY allowed an accurate correction for these experimental effects.

The SAMMY analysis of the experimental data was performed sequentially; the parameter covariance matrix obtained from the analysis of one experimental sequence was used as input in the analysis of the next sequence. A Gaussian function with an exponential tail was used for the experimental resolution function. Most of the components of the resolution function were well known, except the so-called exponential folding width which was obtained from preliminary analysis of well-isolated p-wave resonances at different neutron energy.

Two fictitious large negative resonances and two fictitious large resonances above 125 keV were used for the contribution of the external resonances. The parameters of the fictitious resonances were obtained from preliminary analysis of Harvey transmission data with the value of 5.365 fm for the effective scattering radius R′.

3. Results of the analysis: the resonance parameters

3.1 Level spacing and neutron strength function

The spin and parity of ^{55}Mn is $5/2^-$. The capture of s-wave neutrons would populate compound state of spin J = 2^- and 3^-, and p-wave neutron would populate compound states of spin J = 1^+, 2^+, 3^+, and 4^+. In the energy range 0 to 125 keV, 45 s-wave resonances and 117 p-wave resonances were used to describe the cross sections. Spin assignments for the s-wave resonances were essentially those of earlier works. Because the spin assignments for the p-wave resonances are not possible from the available experimental data, the p-wave resonances were distributed in six groups of non-interfering resonances, at random, according roughly to the J dependence of the level density with a spin cut-off factor $\sigma = 3.5$.

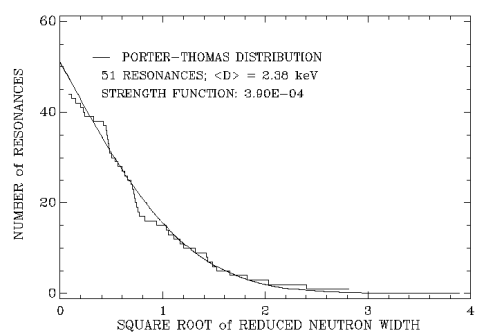

Fig. 1. Integral distribution of the s-wave reduced neutron widths.

The integral distribution of the reduced neutron widths, $g\Gamma_n^0$, of the s-wave resonances is given in Fig. 1. The histogram represents the experimental values, and the solid line is the Porter-Thomas distribution normalized to 51 values, assuming that six small $g\Gamma_n^0$ values are missing. The corresponding average level spacing and neutron strength function are the following, respectively:

$D_0 = 3.80 \pm 0.20$ keV and
$S_0 = (3.90 \pm 0.78) \times 10^{-4}$

The integral distribution of the reduced neutron width, $g\Gamma_n^1$, of the p-wave resonances is given in Fig. 2. Assuming that the average value is independent of the spin J of the resonances, the experimental distribution should correspond to a Porter-Thomas distribution. However, the figure shows an excess of small values, which means that a large number of these small values pertain to d-wave resonances. The experimental histogram corresponding to the $g\Gamma_n^1$ values larger than 0.01 eV can be roughly fitted by a Porter-Thomas distribution normalized to 92 values. Consequently, 25 resonances should be d-wave resonances. The corresponding values of the p-wave level spacing and strength function are the following, respectively:

$D_1 = 1.32 \pm 0.28$ keV and
$S_1 = (0.45 \pm 0.08) \times 10^{-4}$

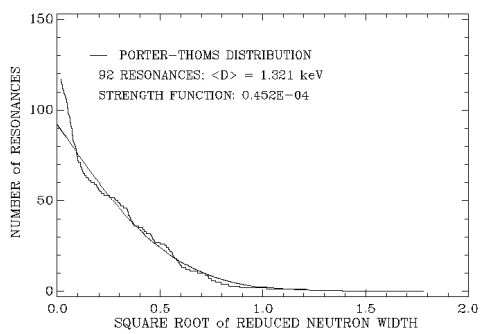

Fig. 2. Integral distribution of the p-wave reduced neutron widths.

Comparison between the s-wave strength function obtained in the present work with earlier results is given in Table 1. The errors are the sampling errors corresponding to the number of resonances in the given energy ranges. The differences between the results are due to the experimental and analysis uncertainties. The value from Saclay (Morgenstern, 1967) agrees with the present results. The value from Rohr et al. (1967), GELINA, is 20% smaller, and the value from Garg (1978), Columbia, is 12% larger.

Only one value of the p-wave strength function, obtained from the resonance parameters, is found is the earlier works. It is the value of Garg and Macklin (1978) obtained from the analysis of capture cross section measured at ORELA in 1978. Their value of $S_1 = (0.35 \pm 0.05) \times 10^{-4}$ is 29% smaller than the value proposed in the present work. Part of the disagreement is due to a nuclear radius of 4.5 fm used by Garg and Macklin to calculate the reduced neutron widths from the measured neutron widths, compared to the value of 5.365 fm used in the present work. Using 4.5 fm instead of 5.365 fm has an effect of decreasing the reduced neutron width by 16% at 10 keV neutron energy and by 3% at 100 keV.

Table 1
Comparison of the s-wave strength function ($S_0 \times 10^4$) obtained in the present work with earlier values obtained in the same energy ranges

Energy (keV)	This work	Saclay (1967)	Rohr (1967)	Garg (1978)
17–75	4.28±1.2	4.14±1.4		
0–100	3.81±1.1			4.26±0.65
50–100	2.45±0.9		2.03±0.77	

3.2 The average capture widths

The s-wave resonances have neutron width values Γ_n generally much larger than the capture width Γ_γ. Therefore, Γ_γ is fully determined by the experimental capture area with the accuracy of the capture area. The average of the 45 values in the energy range 0 to 125 keV is 565 ± 28 meV, which compares to the value of 713 ± 150 meV proposed by Garg and Macklin (1978) from the analysis in the energy range 4 to 110 keV. The Γ_γ of the first three s-wave resonances (energy range 0.05 to 4 keV) was evaluated by Macklin (1985) in 1984 from a capture measurement using thin samples to minimize the experimental effects. He obtained values which are on average 70% smaller than the present values. Since the capture cross sections analyzed in the present work were obtained with thicker samples, resulting in much stronger multi-scattering effects, the difference could be due to inaccurate calculation of the experimental effects by SAMMY. The SAMMY fit of ORELA experimental capture data in the energy range 0.05 to 4 keV is displayed in Fig. 3; the three s-wave resonances seem to be doublets due to the strong multiple scattering effect. Nevertheless the fit is reasonably good. This case has been specially examined by one of the authors (N. M. Larson), who concludes that at least 10% accuracy is achieved on the parameters.

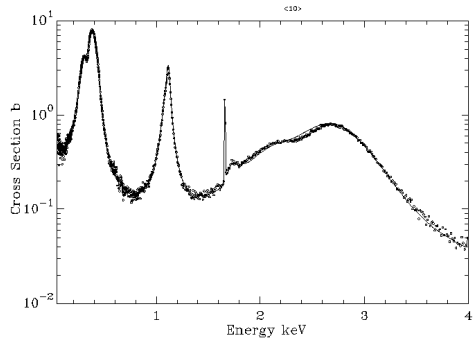

Fig. 3. SAMMY fit of ORELA experimental capture cross sections in the energy range 0.05 to 4 keV. The solid line represents the cross section calculated by the resonance parameters.

The Γ_n and Γ_γ of the p-wave resonances are, for most of them, of the same order of magnitude. In a Bayesian sequential analysis, analyzing first the transmission data will determine the Γ_n values which are proportional to the total area of the resonances, independently of the experimental resolution. If the next sequence is an experimental capture, Γ_γ will be determined by the capture area, which is proportional to $\Gamma_n\Gamma_\gamma/(\Gamma_n+\Gamma_\gamma)$, independently of the experimental resolution. Actually, the transmission data analyzed in the present work has poor statistical accuracy. Most of the p-wave resonances seen in the experimental capture do not emerge from the statistical fluctuations of the transmission. Therefore, the Γ_n values are poorly determined, or not determined, by the transmission data. The solution of keeping Γ_γ at a pre-evaluated constant value gave poor fit of the experimental data. In the present work both Γ_n and Γ_γ were allowed to vary for most of the p-wave resonances. Since the final values of Γ_γ did not fluctuate too much around a realistic average value of 422 meV, it has been assumed that the parameters were determined with reasonable accuracy.

The average value of 422 ± 50 meV for the capture widths of the p-wave resonances agree with the value of 400 ± 100 meV proposed by Garg and Macklin (1978). Note that the spin J of the p-wave resonances were randomly assigned, and it is $g\Gamma_\gamma$ which is really determined. The uncertainty of 50 meV on the average value takes into account this possible cause of error.

4. Results of the analysis: the cross sections

4.1 The thermal range

The results of the SAMMY fit in the low neutron energy range are displayed in Fig. 4. The solid line represents the cross sections calculated by the resonance parameters. The calculated values at 0.0253 eV are the following:

Total cross section: σ_t = 15.39 b
Capture cross section σ_γ = 13.27 b
Elastic cross section σ_n= 2.12 b

These values can be adjusted by small variation of the parameters of the resonance at -759.81 eV. The value of 13.27 b for the capture cross section has been obtained by averaging $\sigma_\gamma E^{1/2}$ in the experimental data of Widder (1975) in the energy range 0.024 to 0.027 eV. On the other hand, the weighted average of all the measurements at 0.0253 eV is 13.24 ± 0.12 b.

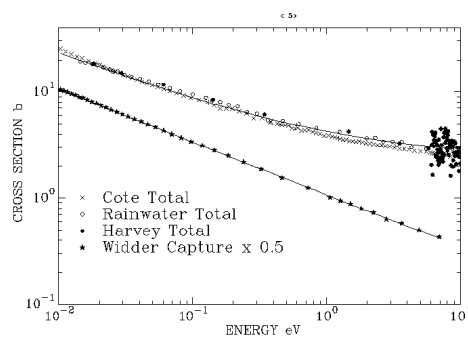

Fig. 4. SAMMY fit of the experimental total cross sections and of the experimental capture cross section in the energy range 0.01 to 10 eV. The solid line represents the cross section calculated by the resonance parameters.

4.2 The resolved resonance region

Examples of SAMMY fits in the resolved resonance region are given in Fig. 5 and Fig. 6, showing the total cross section obtained from the experimental transmission of Harvey (2007), the ORELA and the GELINA effective capture cross sections, in the energy ranges of 30 to 40 keV and 80 to 100 keV, respectively.

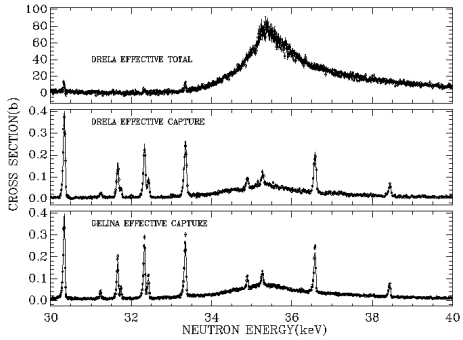

Fig. 5. SAMMY fit of the experimental total cross sections and of the experimental capture cross sections in the energy range of 30 to 40 keV. The solid line represents the cross section calculated by the resonance parameters.

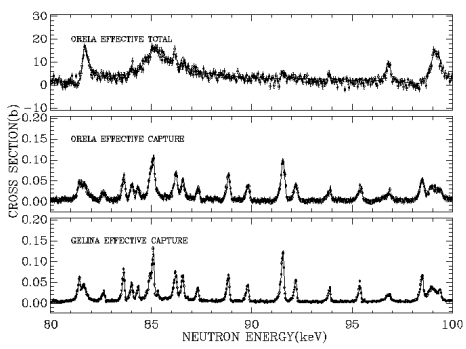

Fig. 6. SAMMY fit of the experimental total cross sections and of the experimental capture cross section in the energy range of 80 to 100 keV. The solid line represents the cross section calculated by the resonance parameters.

The ORELA experimental capture cross sections were normalized relatively to the gold capture cross section with 2% accuracy. GELINA data were normalized with an accuracy not known by the author of the present evaluation. Good representation of the experimental cross sections with the resonance parameters was possible with small normalization corrections (less than 2%) but with an important contribution of a smooth background (2 to about 20% of the average cross section, depending on the energy range). The background is larger in GELINA data than in ORELA data. This background could be due to (1) the uncertainties in the evaluation of the experimental background, (2) the contribution of a direct capture component, and/or (3) to the contribution to the d-wave resonant capture. The contributions of possible direct capture and d-wave capture components are shown in Fig. 7. The open stars with error bars represent the result of a statistical model calculation of the total d-wave contribution. The figure shows that the ORELA background could be explained by the direct and/or the remaining d-wave component. It is estimated that this background contribution is known with 30% accuracy, which is the main component of the systematic uncertainty on the average capture cross section.

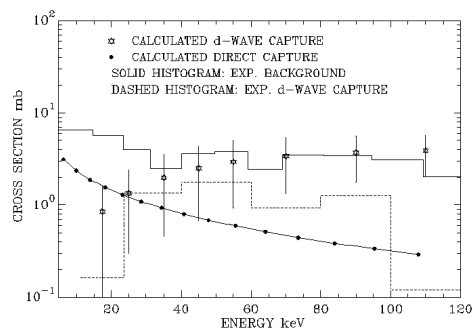

Fig. 7. Background in the capture cross section. The solid histogram represents the background as obtained from the SAMMY analysis of ORELA capture data. The dashed histogram represents the part of the d-wave resonance capture calculated by the identified d-wave resonances.

The flat-weighted average capture cross sections calculated in 18 energy groups are compared to ENDF/B-VII evaluation in Table 2. In the thermal range, the differences are very small. In the energy range of 0.05 to 5.5 keV, the present evaluation is 30% larger due to different evaluation of the capture width of the s-wave resonances. Above 10 keV the differences between ENDF/B-VII and the present evaluation fluctuate strongly, from -16 to 16% depending on the energy range.

Comparison with other experimental data is shown in Table 3. Lerigoleur (1976) values are the results of an absolute measurement. The present evaluation is 12% smaller on average, in the limit of the uncertainties. Garg and Macklin (1978) values are 15% on average larger than Lerigoleur values.

Table 2
Average capture cross sections in barns compared to ENDF/B-VII evaluation

Energy range (keV)	Present results (b)	B-VII (b)	Deviation (%)
1.E-5–3.E-5	15.546	15.619	-0.5
3.E-5–1.E-4	8.630	8.720	-1.0
1.E-4–1.E-3	3.214	3.246	-1.0
1.E-3–1.E-2	1.038	1.037	0.1
0.010–0.050	0.480	0.449	6.9
0.050–0.800	2.840	2.178	30.0
0.800–5.500	0.388	0.292	33.0
5.500–14.00	0.0779	0.0732	6.4
14.00–25.00	0.0443	0.0417	6.2
25.00–30.00	0.0304	0.0352	-16.0
30.00–40.00	0.0252	0.0265	-5.2
40.00–50.00	0.0204	0.0182	12.1
50.00–59.00	0.0199	0.0173	15.0
59.00–68.50	0.0180	0.0196	-8.9
68.50–80.00	0.0162	0.0167	-3.1
80.00–95.00	0.0157	0.0151	4.0
95.00–108.5	0.0120	0.0132	-10.0
108.5–125.0	0.0112	0.0139	-24.0

Table 3
Average capture cross sections compared to other experimental results

Energy Range (keV)	Present Results (mb)	Lerigoleur (1976) (mb)	Garg and Macklin (1978)
15–20	47.98 ± 2.05	57.05 ± 4.56	48.6
20–30	35.79 ± 1.79	40.97 ± 3.28	44.6
30–40	25.24 ± 1.20	27.43 ± 2.19	44.7
40–50	20.44 ± 1.20	19.58 ± 1.57	28.2
50–60	20.40 ± 1.20	20.41 ± 1.63	26.0
60–80	16.69 ± 1.30	20.19 ± 1.61	21.5
80–100	15.00 ± 1.10	17.63 ± 1.41	16.3
100–120	11.63 ± 1.10	12.64 ± 1.01	14.3
15–120	20.24(12%)	22.60(0%)	25.91(15%)

5. Conclusions

The ^{55}Mn resonance parameters were evaluated in the energy range of 0 to 125 keV, below the first inelastic channel, by the SAMMY analysis of the most recent ORELA neutron transmission and ORELA and GELINA capture cross section measurements. The accuracy of the parameters has improved compared to the current Evaluated Nuclear Data File. However, the large thickness of the sample used in the capture measurements caused some difficulties in the analysis of the large s–wave resonances in the low energy range, due to the important multiple scattering effects. It is believed that the code SAMMY calculates these strong experimental effects with a good accuracy, which gives credibility to the capture widths obtained in the present evaluation compared to the values proposed by Macklin. This result should be confirmed by further capture measurements using thinner samples. On the other hand, the poor statistical accuracy of the transmission measurements did not allow accurate evaluation of the neutron widths of the p-wave resonances. Thick sample transmission measurements with high statistical accuracy are needed.

The resonance parameters were converted to the ENDF/B format and added to the higher energy range of the ENDF/B-VII file, with the corresponding Resonance Parameter Covariance Matrix (RPCM). The new file was processed with the code PUFF IV (Wiarda and Dunn, 2006) in the calculation of group cross sections and uncertainties on group cross sections. The infinite dilute resonance integral calculated from the new file is 13.52 ± 0.30 b compared to 13.4 ± 0.5 recommended by Mughabghab, and 13.42 from ENDF/B-VII.

6. Acknowledgement

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References

Cote, R.E., Bollinger, L.M., Thomas, G.E., 1964. Phys. Rev. 144,5B, 1047.

Garg, J.B., Macklin, R.L., and Halperin, J., 1978. Phys. Rev. 18C, 5, 2079.

Garg, J.B., 1978. Nucl. Sci. Eng. 65, 76.

Guber, K., 2007. unpublished, Oak Ridge National Laboratory, Oak Ridge TN, USA.

Harvey, J.A., 2007. Private communication, Oak Ridge National Laboratory, Oak Ridge TN, USA.

IAEA, 1983. World Request List for Nuclear Data, WRENDA 83/84, INDC(SEC)-88/URSF, PIKSAIKIN, V., Ed., Vienna.
Lerigoleur, C., et al., 1976. CEA R-4886, Cadarache, France.
Macklin, R.L., 1985. Nucl. Sci. Eng. 89, 362.
Morgenstern, J., et al., 1967. Nuc. Phy. A102, 602.
Perrot et al., 2003. Nuc. Sci. Eng. 144, 142-146.
Rainwater, L.J., 1947. Phy. Rev. 71, 65.
Rohr, G., Friedland, E., 1967. Nuc. Phy. 104A,1.
Shillebeeckx, P., 2007. Private communi-cation, Int. for Ref. Mat. And Meas. (IRMN), Geel, Belgium.
Wiarda, D.A., Dunn, M.E., 2006. ORNL/TM-2006/147, Oak Ridge National Laboratory, Oak Ridge TN, USA.
Widder, F., 1975. R-EIR-217, Inst. For Reactor Physics, Wuerenlingen, Switzerland.