Narrow beam neutron transmission benchmarks and evaluated data in the region of resonance cross section structures

V.G. Pronyaev, O.N. Andrianova, V.V. Sinitsa INDEN CM on Evaluated Data for Structural Materials IAEA, Vienna, 16 – 20 December 2024

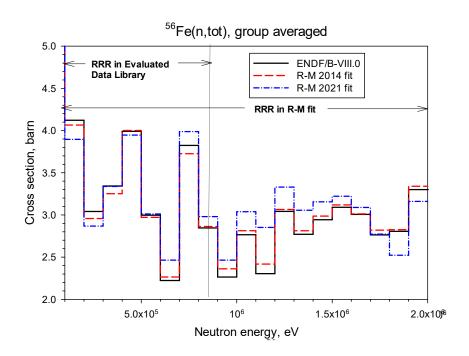
# **Evaluations**

High resolution measurements show that the resonance type structures exists in the structural material cross sections up to the energy at 5 MeV.

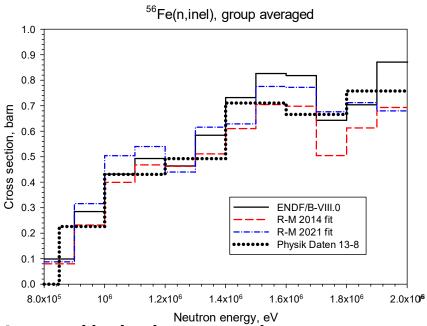
At present evaluated data libraries, the Resolved Resonance Range (RRR) for best studied <sup>56</sup>Fe is extended up to the threshold of first inelastic level – 850 keV (REFIT, F. Froehner and F. Fabbri, 1992) with some minor modifications. For higher energies, the cross sections are presented with the resonance type structures taken from available high-resolution measurements.

Attempts to extend the RRR up to 2 MeV (energy below the threshold of second inelastic scattering level) were made by L. Leal (2014 and 2021, SAMMY). The R-M parameters included the widths for elastic, capture and inelastic channels. The main problem is that the experimental resolution is not enough to identify the narrow resonances. As result, they can be missed in the fit. This causes some problems in the description of the observed average capture and to less extent – elastic scattering cross section. The smooth background cross sections are usually added as option to compensate the missed resonances.

## **Evaluations**



Averaged total cross sections: ENDF/B-VIII.0 RRR to 850 keV, high-resolution experimental data above R-M2014, R-M2021 – RRR to 2 MeV



Averaged inelastic cross sections: ENDF/B-VIII.0 high-resolution experimental data R-M2014, R-M2021 – RRR to 2 MeV Physik Daten (1992) – LSQ combined fit of experimental data (n,tot), (n,el), (n,inl), (n,γ)

# **Evaluations**

### Data used in the R-M (2021) fit of <sup>56</sup>Fe+n cross sections

To benchmark	Energy Range	Facility	TOF (meters)	Measurement
Harvey (1987)	20 keV – 2 MeV	ORELA	201.575	Transmission
Perey (1990)	120 keV – 850 keV	ORELA	201.575	Transmission
Cornelis (1982)	500 keV – 2 MeV	GELINA	387.713	Transmission
Danon (2012), 3 thicknesses	500 keV – 2 MeV	RPI	249.740	Transmission
Perey (1990)	850 keV – 1.5 MeV	ORELA	201.575	Inelastic
JRC/GEEL (2011)	850 keV – 2 MeV	GELINA	198.686	Inelastic
Spencer (1994), 2 thicknesses	10 eV – 650 KeV	ORELA	40.0	Capture
Perey (1990)	850 keV – 1.5 MeV	ORELA	200.191	Elastic
Cabé (1967)	500 keV – 1.2 MeV	Univ. de Louvain (Van de Graaff)	~ 1	Elastic

## **Benchmark: Transmission and Effective Cross Section**

Latest description of the narrow beam transmission measurements (FUND-IPPE-VdG-MULT-TRANS-001) done in the IPPE in 1960-th at IPPE (Non-exponentiality of Neutron Transmission, by G.B. Lomakov, M.N. Nikolaev and V.V. Filippov is published in Yadernye Konstanty, p. 148, issue 1 (2016). Measurements were done at 2 VdG accelerators with proton on tritium neutron source and were continued few years (50 energy ranges times 27 sample thicknesses). It is unrealistically to repeat the measurements with this method at present.

Measured transmission T(t) for homogeneous sample according to the measurement conditions:

$$T(t) = \int_{E_i}^{E_{i+1}} R(E) \exp\left[-\sigma(E)\rho t\right] dE$$

R(E) – resolution function normalized at 1 in the energy group  $(E_i, E_{i+1})$ 

```
\rho - sample nuclear density, t - sample thickness, \tau = \rho t - nuclear thickness in nuclei/barn
```

 $\sigma(E)$  – microscopic total cross section

If introduce effective cross section for given thickness  $\sigma_{eff}(t)$ , which is constant and describes the transmissio in the energy group  $(E_i, E_{i+1})$ , then

 $T(t) = exp[-\sigma_{eff}\tau]$ 

 $\sigma_{\text{eff}}(t) = -\ln T(t)/\tau$ 

# **Benchmark: Uncertainty**

The paper contains analysis of uncertainties of measurements caused by different factors:

- 1. Uncertainty in the shape and boundaries of resolution function
- 2. Uncertainty in neutron flux monitoring
- 3. Uncertainty in the room return background
- 4. Uncertainty in the sample thickness
- 5. Statistical uncertainty

Correction at multiple scattering contribution was small and not considered, but the comparison of experimental results will be done with MC calculations, which account the neutron multiple scattering.

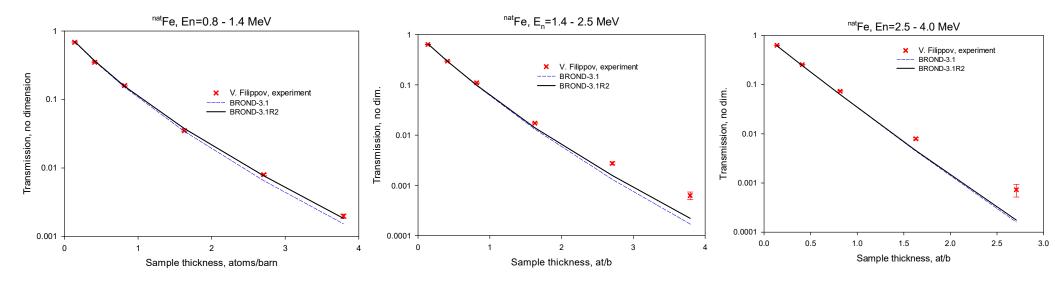
Total uncertainty assigned to the measured transmission is for most energy groups between 1 - 2% (thin samples) and 10 - 20% (thick samples).

Relative uncertainty of effective cross section for small thicknesses can be 10-15% and a few % for large thicknesses due to (*InT*) term in the denominator of

$$\frac{\sigma_{eff}}{\sigma_{eff}} = \sqrt{\left(\frac{\Delta\tau}{\tau}\right)^2 + \left(\frac{\Delta\tau}{T}\right)^2 / (lnT)^2}$$

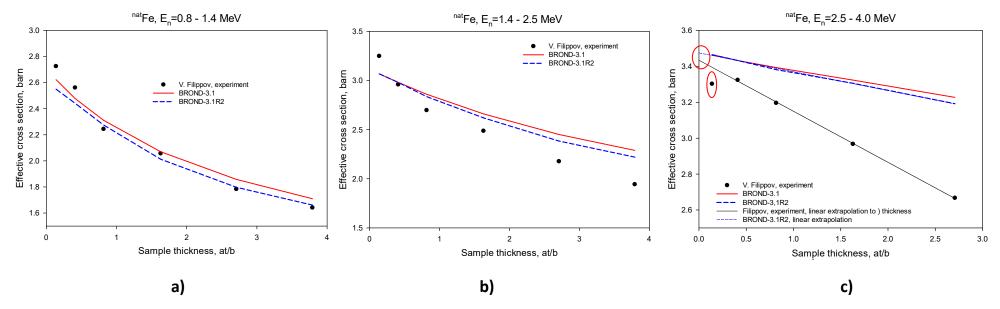
# Comparison of experimental and calculated results for <sup>nat</sup>Fe in wide energy groups: transmission

MC calculations of natural iron transmission for BROND-3.1 (RRR to 850 keV, above – high resolution experimental data data) and BROND-3.1R2 (RRR up to 2 MeV - R-M 2021 evaluation, above – high-resolution experimental data). Cross sections for other iron isotopes are taken from BROND-3.1 library.



Conclusion: good consistency for 0.8 – 1.4 MeV group, underestimation of resonance structure in evaluations for more high-energy groups.

## Comparison of experimental and calculated results for <sup>nat</sup>Fe in wide energy groups: effective cross-section

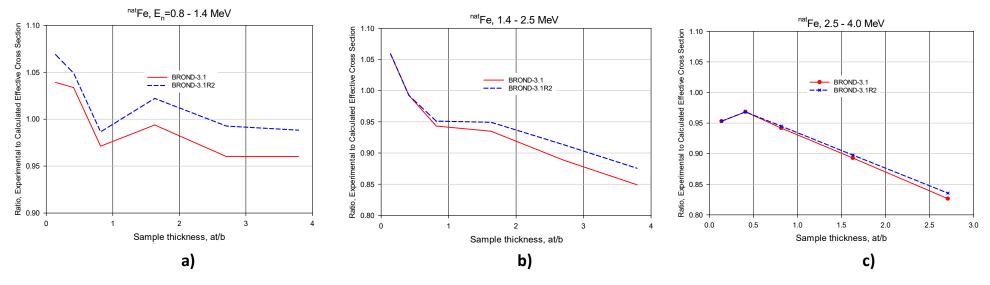


Effective cross section in the limit of 0 sample thickness is equal to the average cross section.

Effective cross section in the limit of the infinite large sample thickness is equal to the minimal cross section.

Interpretation for evaluations: a) average cross section is underestimated, resonance structure is consistent; b) average cross section and resonance structures are underestimated; c) average cross section is slightly overestimated, resonance structure is underestimated; transmission measurements problems for small thicknesses.

### Comparison of experimental and calculated results for <sup>nat</sup>Fe in wide energy groups: ratio of effective cross-section



Ratio of experimental to calculated effective cross section with account of their uncertainties is most informative. Interpretation for evaluations:

- a) average cross section is practically consistent, resonance structure is better consistent for BROND-3.1R2;
- b) average cross section is consistent and resonance structures are underestimated;
- c) average cross section is consistent, resonance structure is strongly underestimated;

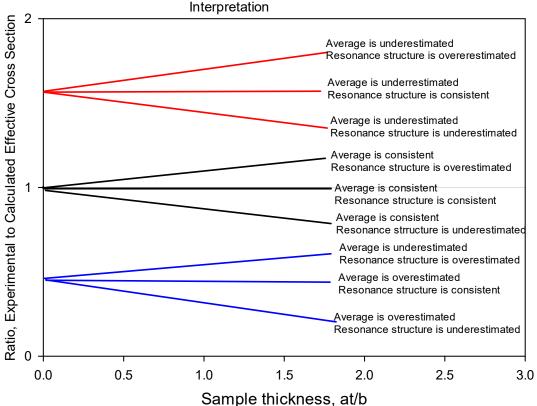
There are clear transmission measurements problems for small sample thicknesses.

## **Comparison of experimental and calculated results: interpretation of the effective cross section ratios**

Taking into account, that:

- 1. effective cross section for small sample thickness tends to average cross sections
- 2. effective cross section for large sample thicknesses tends to the cross sections in the minima

The following interpretation of experimental to calculated effective cross section ratios can be used:



## **Detailed comparison (50 energy ranges with 27 thicknesses)**

The comparison is shown for the most characteristic energy ranges:

4 – 43 keV – near left border of resonance range, first s-resonance minimum, 291 – 329 keV – near the middle of usual standard resonance ranges, strong transmission over-prediction;

575 – 880 keV – end of usual resonance range, clear problems with experimental data for thicknesses less than 5 cm;

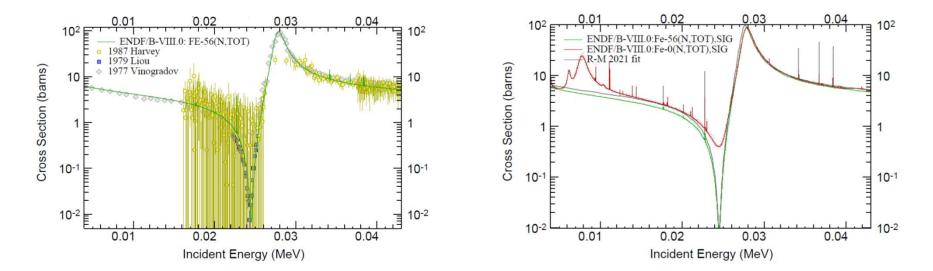
874 – 1160 keV – just above the usual resonance range and threshold of inelastic scattering

**2.26 – 2.45** MeV – high-resolution experimental data are used in all libraries, strong underestimation of resonance structures

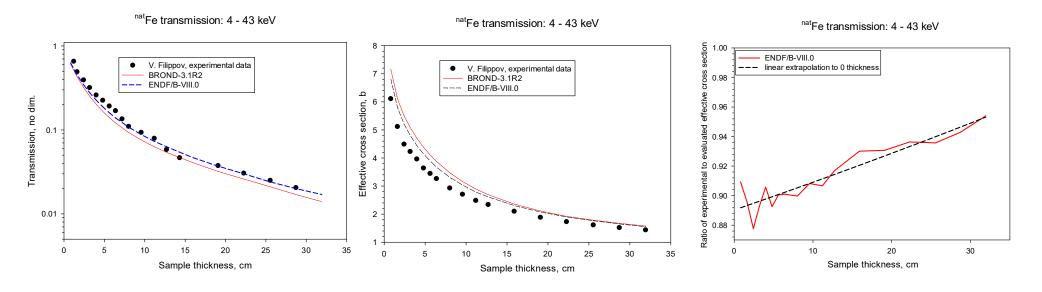
**3.407** – **3.560** MeV - end of high-resolution and neutron transmission data, strong underestimation of resonance structures.

### Detailed comparison: 4 – 43 keV range

4 – 43 keV range includes prominent 24 keV resonance. It has strong interference minimum. ENDF/B-VIII.1 has contribution from direct capture increasing the total cross section in the minimum at few mb. This revision has no practical influence at the <sup>nat</sup>Fe transmission



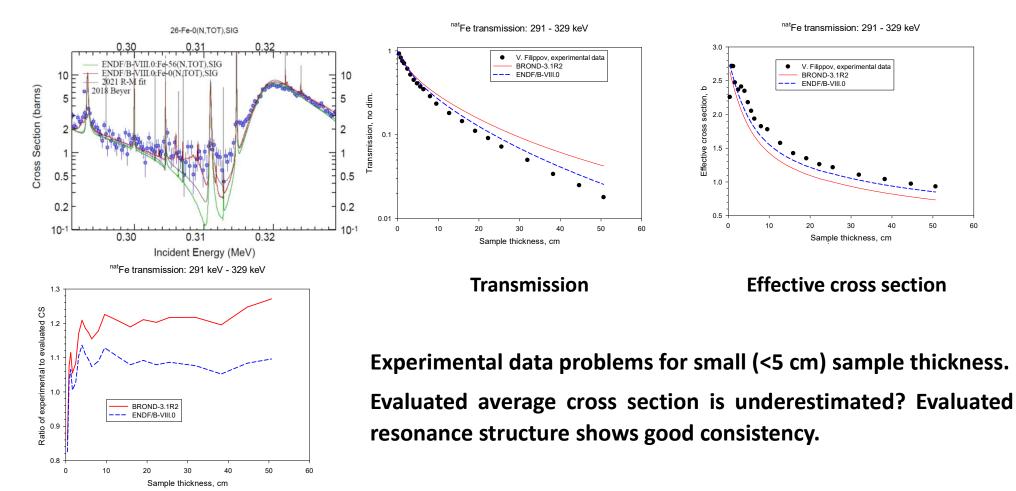
### **Detailed comparison: 4 – 43 keV range**



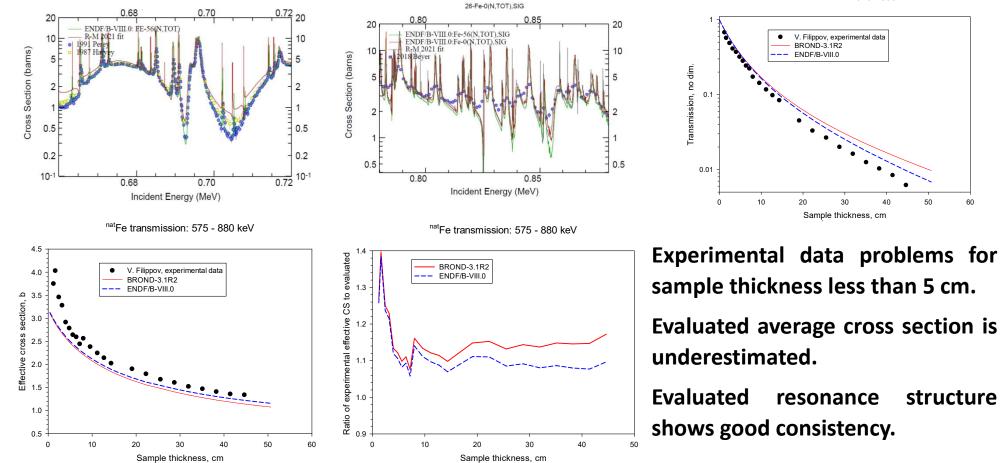
TransmissionEffective cross sectionRatio of effective cross sectionsEvaluated average cross section is underestimated at 12%?

**Evaluated resonance structure is overestimated?** 

### Detailed comparison: 291 – 329 keV range



### Detailed comparison: 575 – 880 keV range



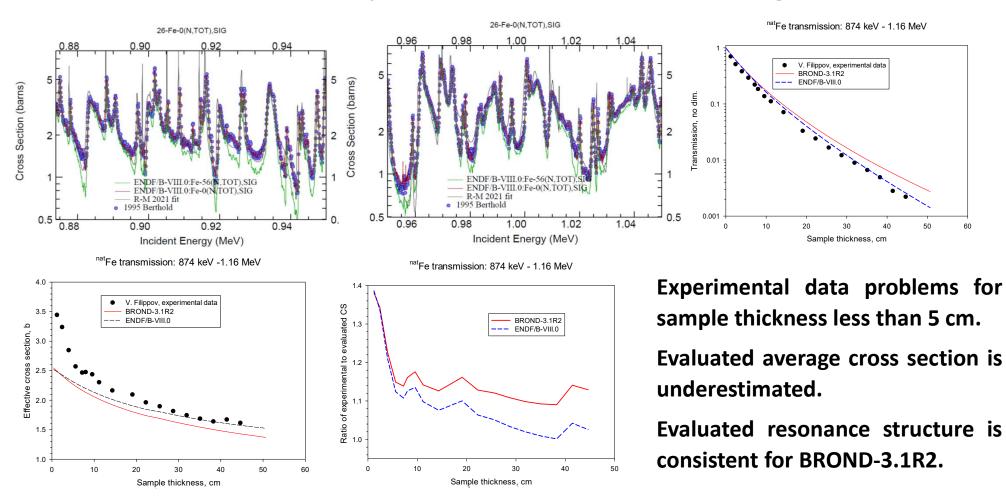
<sup>nat</sup>Fe transmission: 575 - 880 keV

50

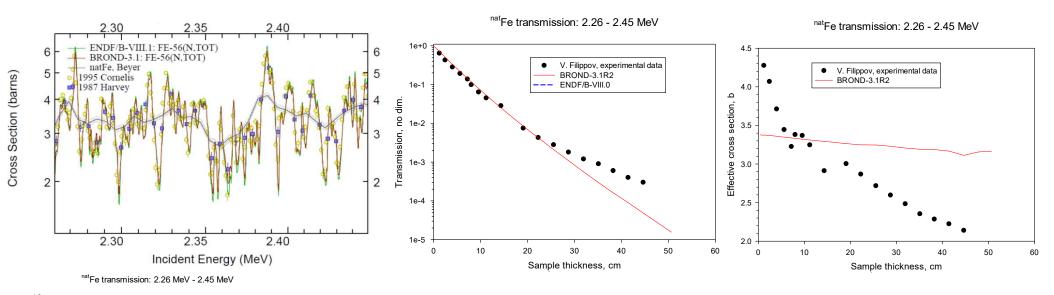
60

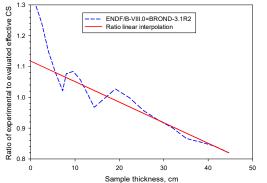
structure

### Detailed comparison: 874 – 1160 keV range



### Detailed comparison: 2.26 – 2.45 MeV range

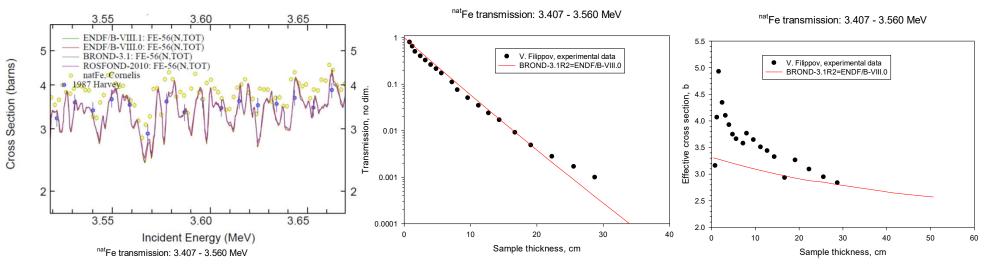


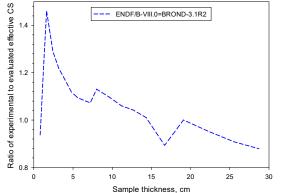


Experimental data problems for sample thickness less than 5 cm. Evaluated average cross section is underestimated.

Evaluated resonance structure is strongly underestimated.

### Detailed comparison: 3.407 – 3.56 MeV range





Experimental data problems for sample thickness less than 5 cm. Evaluated average cross section is underestimated.

**Evaluated resonance structure is strongly underestimated.** 

### **General conclusion**

**1**. Experimental data are not reliable for sample thicknesses less than 5 cm for all energy ranges.

2. Group averaged cross sections are either too high in the measurements, or too low in the evaluations.

3. The spread of the evaluated total cross sections in different R-M fits is between 2 and 15%. It depends from many factors, such as the width of the energy range in the fit, energies and widths of the negative and positive remote resonances, missed resonances.

4. Evaluated resonance structure of <sup>nat</sup>Fe is overestimated in the evaluated data in the region of 24 keV resonance in <sup>56</sup>Fe.

5. Evaluated resonance structure is generally consistent with the experimental data in the RRR below 850 KeV.

6. Evaluated resonance structure consists better with experimental when RRR is extended up to 2 MeV.

7. Evaluated resonance structure is underestimated strongly for the energies above 2 MeV if highresolution experimental data are used for its introducing in the evaluated cross sections.

8. New measurements (low resolution TOF) of the neutron transmission in the condition of narrow beam are required. Mono-isotopic (e.g. <sup>55</sup>Mn or <sup>59</sup>Co) and many-isotopic (e.g. Ni) samples can be used for testing of the measurement conditions and method.