Nuclear Data Evaluation Status for Tungsten Isotopes $^{182\text{-}184,186}$W and ^{63,65}Cu

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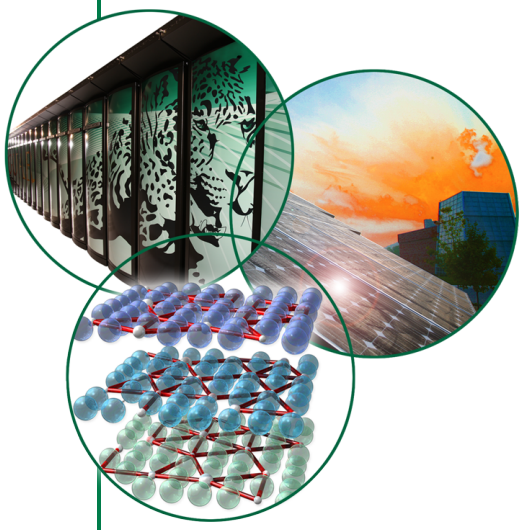

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Outline

- Nuclear Data Evaluation Overview
- Evaluation Procedure with SAMMY
  - Details on the differential data evaluation procedure (cross section from resonance parameters)
  - Link to benchmarks (integral data)
- Evaluation work on ^{183}W (Pigni)
- Evaluation work on ^{182,184,186}Tungsten isotopes (Leal)
- Evaluation work on ^{63,65}Cu (Sobes)

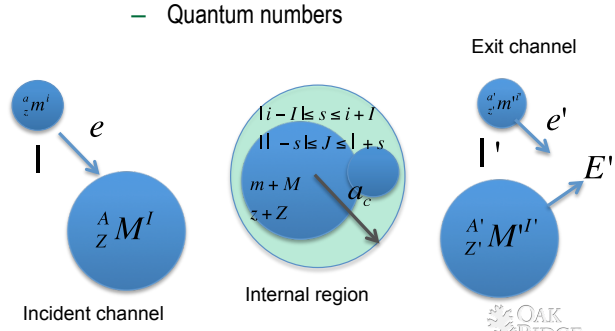
Nuclear Data Evaluation Status Overview

Resolved Resonance Region (RRR) Cross Section Evaluations							
No.	**Nucleus (I^{π})**	$E_{\min} - E_{\max}^{ORNL}(E_{\max}^{existing})$	**Method**	**No. Levels**	**J_0**	**J_1**	**Evaluator**
1	^{182}W (0^+)	10^{-5} eV – 10 (5) keV	RM	143	143	0	L. C. Leal
2	^{183}W ($1/2^-$)	10^{-5} eV – 5 (2.2) keV	RM	339	239	100	M. T. Pigni
3	^{184}W (0^+)	10^{-5} eV – 10 (4) keV	RM	125	125	0	L. C. Leal
4	^{186}W (0^+)	10^{-5} eV – 10 (8.3) keV	RM	78	78	0	L. C. Leal
5	^{63}Cu ($3/2^-$)	10^{-5} eV-300 (100) keV	RM	527	323	204	V. Sobes
6	^{65}Cu ($3/2^-$)	10^{-5} eV-300 (100) keV	RM	762	525	237	V. Sobes

RM – Reich-Moore Approximation

Formalities

- **ORNL Sammy code used to prepare nuclear data evaluations**
  - **In order to directly compare the cross sections extracted from experiments to those generated via any theory one needs**
    - Experimental conditions
      - Doppler broadening
      - Multiple-scattering effects
      - Self-shielding effects
      - Multiple isotopes
      - Resolution function of the facility
      - Sample thickness
    - Theoretical aspects
      - R-Matrix theory
        - Reich-Moore approximation
        - Multi- or single-level Breit-Wigner
      - Quantum numbers

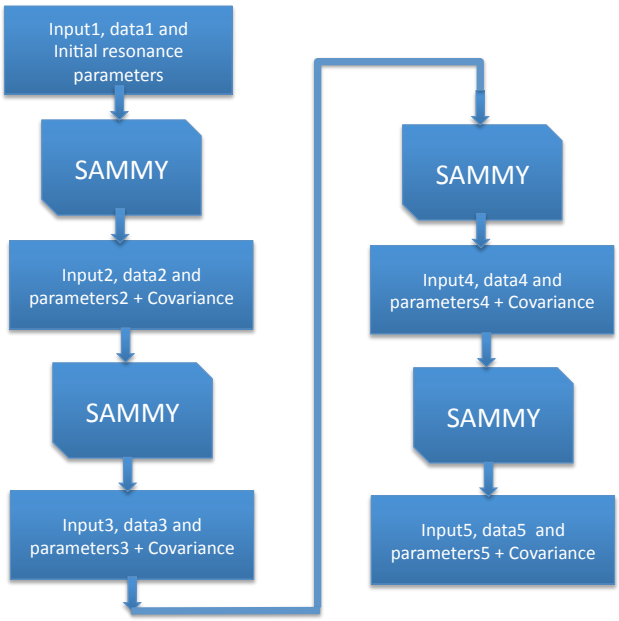


Formalities continued

- SAMMY evaluation procedure requires
  - Experimental data measured at ORELA, GELINA, RPI, or any data available in the EXFOR library
    - For tungsten evaluations only experimental data from GELINA and ORELA have been used
  - Experimental conditions for a consistent SAMMY evaluation provided by K. Guber
  - Initial resonance parameters
    - RSAP and SUGGEL codes may be used to generate a initial set of resonance parameters
    - Existing parameters in major ENDF libraries (ENDF/B-VII.1, JENDL4.0, etc.)

SAMMY Evaluation Procedure (differential data analysis)

SAMMY Sequential Evaluation



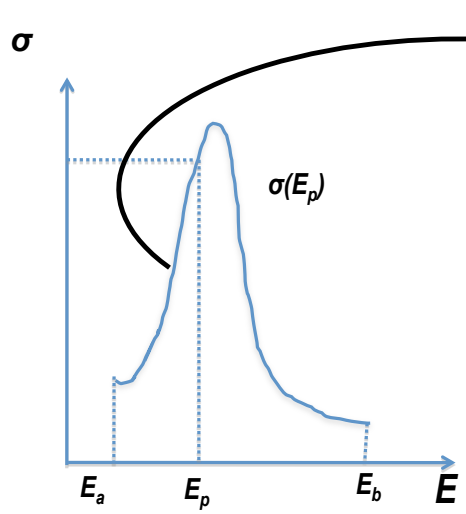
- A final set of parameters should fit reasonably well (small chi-square) the set of experimental data (e.g., data1, data2, data3, data4, data5)
- Generally there are multiple issues to be addressed by the evaluator:
  - Experimental data have different resolution
  - Experimental data have different energy range. Careful analysis of external levels is needed
  - Normalization of experimental data
  - Wrong spin assignment of resonance parameters
  - Missing information in old experiments

SAMMY Evaluation Procedure (link to Integral data)

- All experimental data have been reasonably represented by a set of resonance parameters and covariance (uncertainty) is obtained
  - SAMMY resonance parameter and covariance are converted into the ENDF/B format - file 2 (parameter) and 32 (covariance matrix)
- Process ENDF/B file with NJOY or AMPX in order to generate cross section in pointwise and/or group representation
- Find in the ICSBEP database integral benchmark experiments sensitive to the data of the evaluated isotope(s)
- Run MCNP and/or KENO codes
  - sensitivity analysis using TSUNAMI and TSURFER in order to improve agreement with benchmark experiments
  - Goal: improve results of integral data calculations and, at the same time, have reasonable description of differential data
- SAMMY analysis together with TSUNAMI/TSURFER is the way to go

SAMMY Evaluation Procedure (link to Integral data)

Differential and Integral



σ(E) as a function of energy

$$R = \int_{E_a}^{E_b} \sigma(E)\varphi(E) \quad dE$$

R is the reaction rate (measured quantity)

Differential

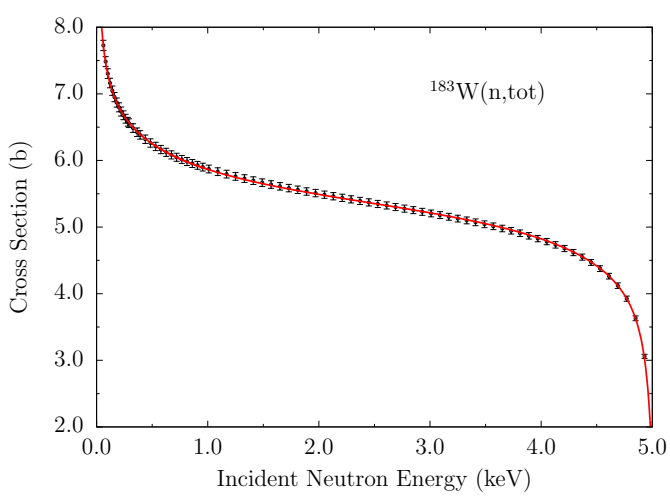
Integral

Starting Point: External Levels and Database

- External levels: bound levels (negative resonances) and levels above the resonance region
  - Careful determination of the external levels is needed before starting a SAMMY evaluation
  - It provides a good understanding of the scattering potential cross section
  - Indicates whether background effects a properly calculated
  - (Effective) nuclear scattering radii are well defined once the external levels have been determined
  - Provides an insight whether a direct reaction component is present
- Consistency of the database
  - Resolution function (ORELA, GELINA, …)
  - Data normalization
  - …

External Levels Evaluation

Contribution from the external levels - bound levels (negative resonances) and levels above the resonance region - and potential scattering cross section



- At low energies the effective radius is well defined and the potential scattering cross section is depending by the channel radius, a, and distant-level parameter, R∞, as

$$\sigma^{pot} \xrightarrow{E->0} 4\pi a^2 (1 - R^{\infty})^2 = 4\pi R'^2$$

- R∞(E) is essentially the difference between the contribution to the R-matrix from the resonances below and above E
- External levels important to avoid troublesome edge effects near the boundaries of the internal region

Figure 1. The potential scattering cross section calculated for a channel radius $a_c = 7.3$ fm and a distant-level parameter $\mathcal{R}_c^{J,\infty} = 0$ plus the contribution of 2 bound, i.e., negative levels below and 3 levels above the RRR 5 keV upper limit. The continuous red curve is a fit to the cross sections obtained by extrapolating the known RRR levels below and above the RRR.

^{183}W cross section evaluation (Pigni)

Step 1: Determination of number of partial waves

- The magnitude of the penetrability factors determines the strength of the partial-wave components responsible of the quasi-stationary compound state.

$$\Gamma_{\lambda c} = 2\gamma_{\lambda c}^2 P_l$$

	ℓ	s	J^π	g_J	wave
^{183}W $(1/2^-)$	0	0	0^-	1/4	s
		1	1^-	3/4	
	1	0	1^+	3/4	p
		1	0^+ 1^+ 2^+	1/4 3/4 5/4	
	2	0	2^-	5/4	d
		1	1^- 2^- 3^-	3/4 5/4 7/4	

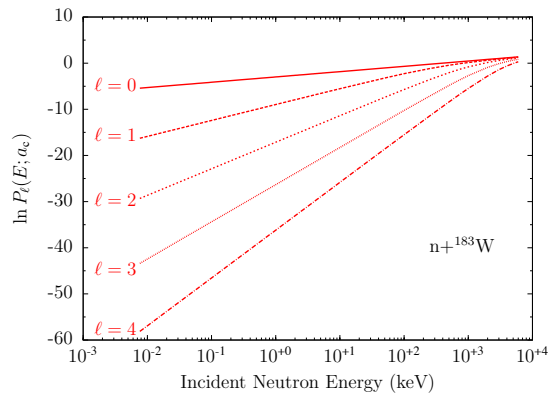
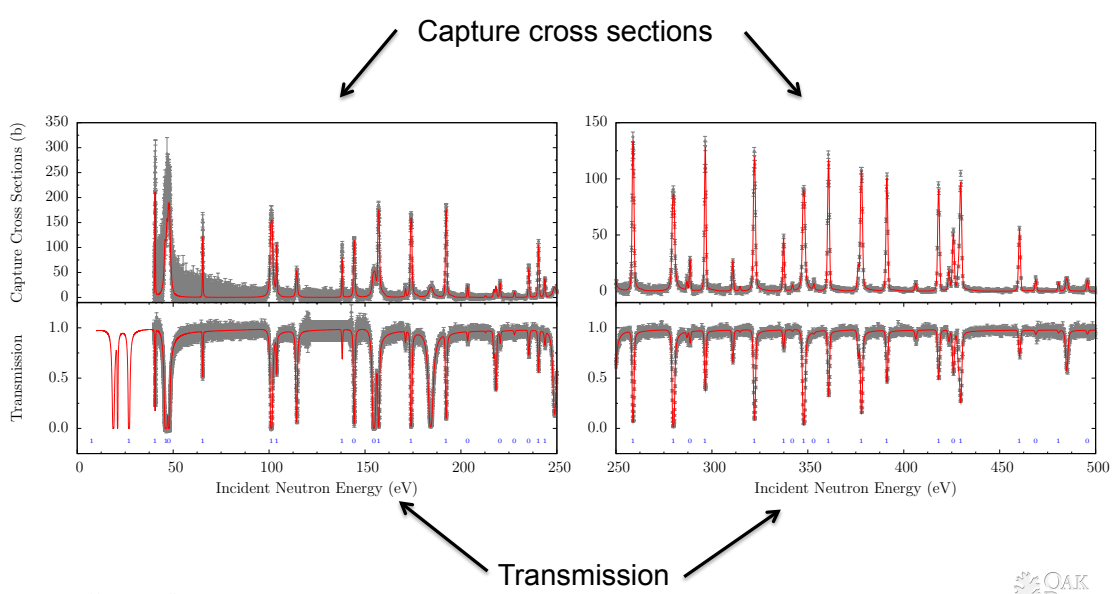


Figure 2. Hard-sphere penetrability factors $P_\ell \equiv P_\ell(E; a_c)$ of n+^{183}W for different angular momentum ℓ calculated at the channel radius $a_c = 7.3$ fm .

^{183}W cross section evaluation (Pigni)

Step 2: Fitting procedure up to 5 keV

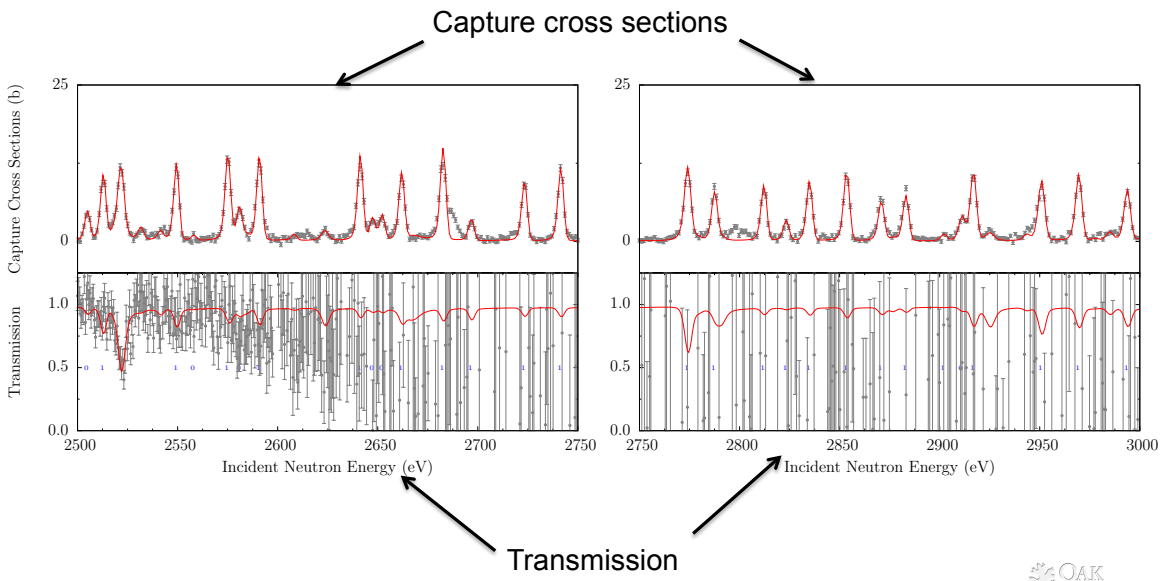
- Since ^{183}W has spin half-integer there are two spin populations for s-wave



^{183}W cross section evaluation (Pigni)

Step 2: Fitting procedure up to 5 keV

- Issue with the experiment for transmission data



^{183}W cross section evaluation (Pigni)

Step 3: Fitting thermal cross section and comparison with major nuclear data libraries

Thermal Cross Sections	Total (b)	Capture (b)	Elastic (b)
This work	12.821	10.406	2.415
JENDL-4	12.815	10.406	2.409
ENDF/B-VII.0	13.427	10.010	3.417
ATLAS	—	10.400	2.400

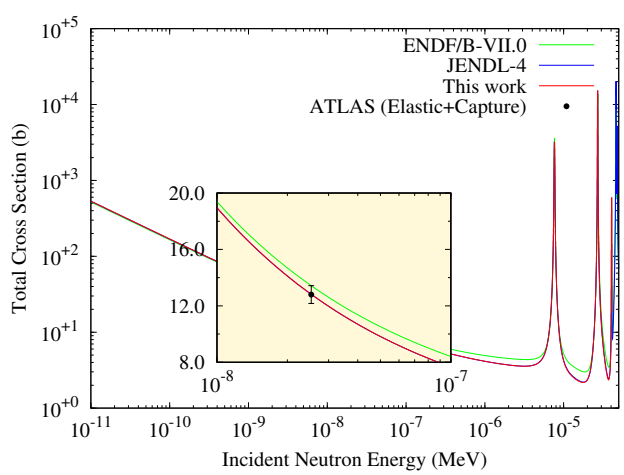
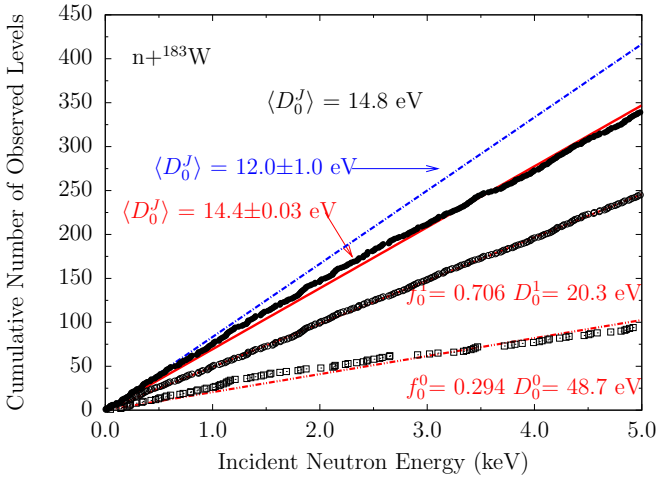


Figure 3. Total cross sections of ^{183}W compared to two major nuclear data libraries. JENDL-4 and the present work are almost identical.

^{183}W cross section evaluation (Pigni)

Step 4: Systematics of resonance parameters



- ^{183}W has two randomly mixed independent spin populations
- Level spacing $\langle D_0^J \rangle$ tends to be smaller than even-A isotopes since there are two spin populations
- Nearly linear slope indicates there are no narrow missed s-levels

Figure 8. Plot of the cumulative number of observed s-levels (black dots) vs energy for n+^{183}W. The values of average s-level spacings for two J-spin populations, $\langle D_\ell^J \rangle$, and the mixed population, $\langle D_0^J \rangle$, shown in the plot represent the inverse of the slope of a straight line fitted to the data (red lines) and obtained by the recommended value (dashed blue line) taken from Mughabghab [9]. The expressions f_0^0 and f_0^1 are the fractional densities of population for $J^\pi = 0^-$ and $J^\pi = 1^-$, respectively.

^{183}W cross section evaluation (Pigni)

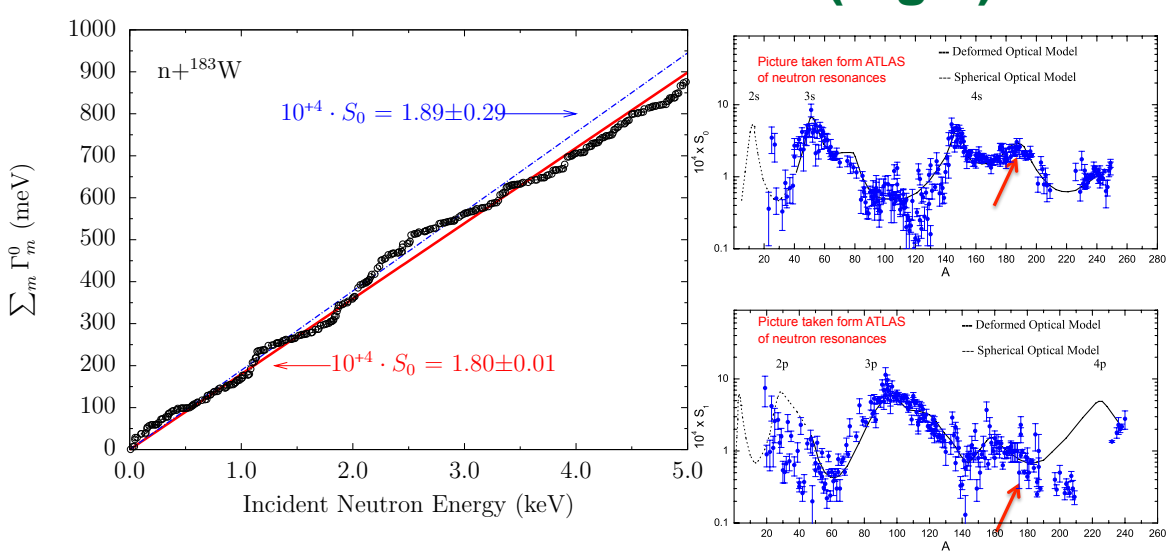


Figure 9. Plot of cumulative reduced neutron-widths $\sum_m \Gamma_m^0$*(open black dots) vs energy for n+^{183}W. The slopes of the straight lines give the strength function S_0 (in 10^{+4} unit). The slope of straight line fitted to the data (continuous red line) and the recommended value taken from Mughabghab [9] (dashed blue line) are shown.

* $\Gamma_m^0 = g_J \Gamma_n^{J,m} \sqrt{1\,\text{eV}/E_m}$

^{183}W cross section evaluation (Pigni)

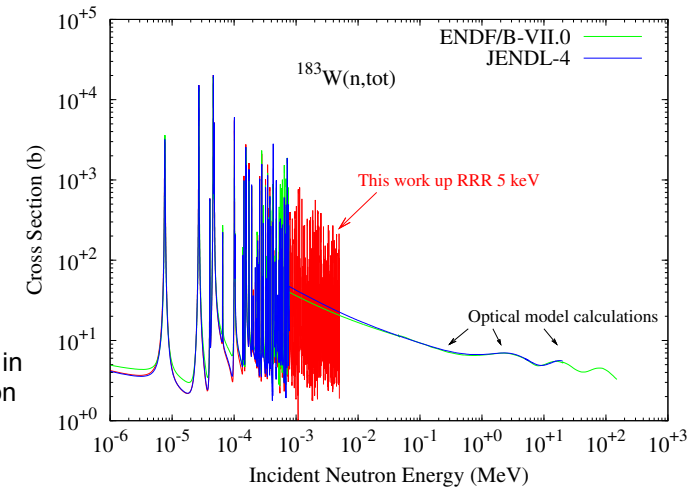
Link resonance parameters to optical model

- The optical model gives cross sections averaged over resonances and the transmission coefficients which are closely related to the strength function

$$T_c \equiv 1 - |\langle U_{cc} \rangle|^2 = \frac{4\pi S_c}{|1 - i\langle R_{cc} \rangle|^2} \frac{\sqrt{E}}{k_c a_c}$$

- The same average can be obtained in R-matrix cross section representation

$$\langle \sigma_c \rangle = \frac{2\pi}{k_c^2} g_c (1 - \mathrm{Re}\langle U_{cc} \rangle)$$



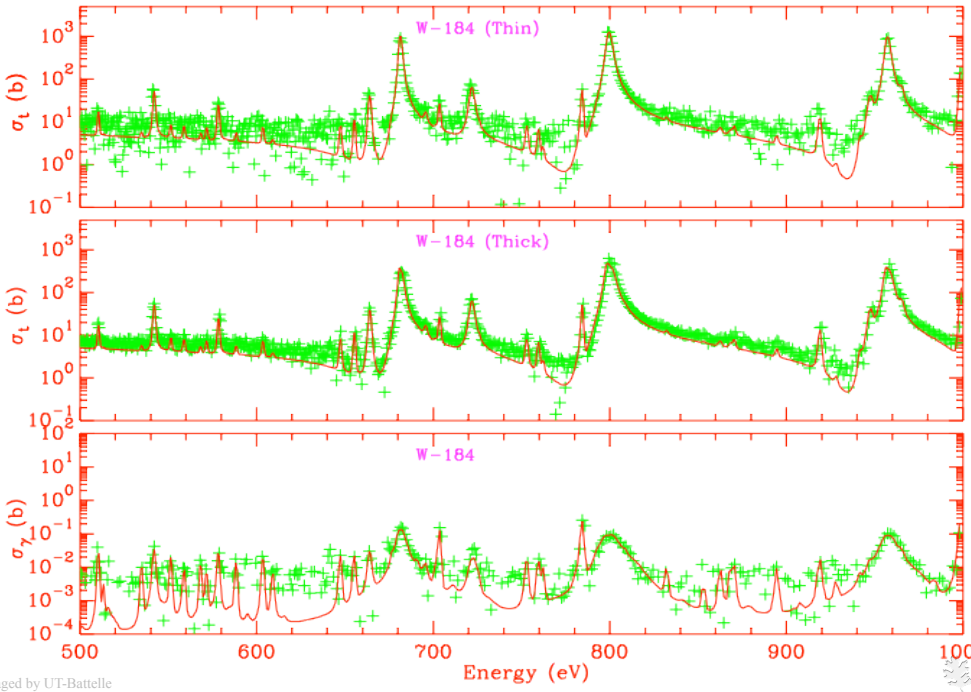
$$\langle U_{cc} \rangle = \frac{I_l(k_c a_c)}{O_l(k_c a_c)} \frac{1 - \langle R_{cc} \rangle (L_l^* - B_l)}{1 - \langle R_{cc} \rangle (L_l - B_l)}, \quad \langle R_{cc} \rangle = R_c^\infty + i\pi S_c \frac{\sqrt{E}}{k_c a_c},$$

Summary ^{183}W Evaluation (Pigni)

- **We have applied the R-matrix SAMMY method using the Reich-Moore approximation to determine a consistent, albeit still preliminary, set of neutron resonance parameters for ^{183}W in the energy range up to 5 keV**
- **In the analyzed energy range, this evaluation doubles the RRR energy range present in the latest US nuclear data library (ENDF/B-VII.1)**
- **The experimental data were used sequentially to ensure that the calculated cross sections were in good agreement for both (n,tot) and (n,γ) reaction channel**
- **We produced preliminary results for the systematics of the observed s-wave resonances, such as level spacing systematics and strength functions**
- **We want to finalize this evaluation of resonance parameters and improve the analysis of their systematics in order to generate consistent assessments of cross-section covariance data**
- **We want to improve optical model potential parameterization**

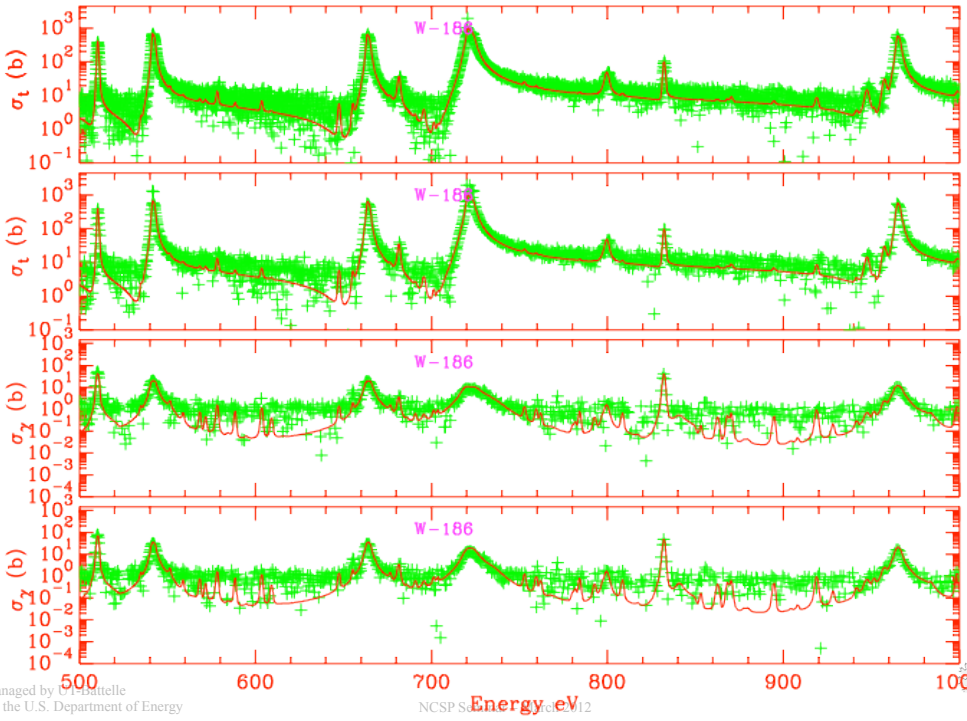
^{184}W cross section evaluation (Leal)

Total and capture cross section for ^{184}W in the energy range 500 eV to 1 keV



^{186}W cross section evaluation (Leal)

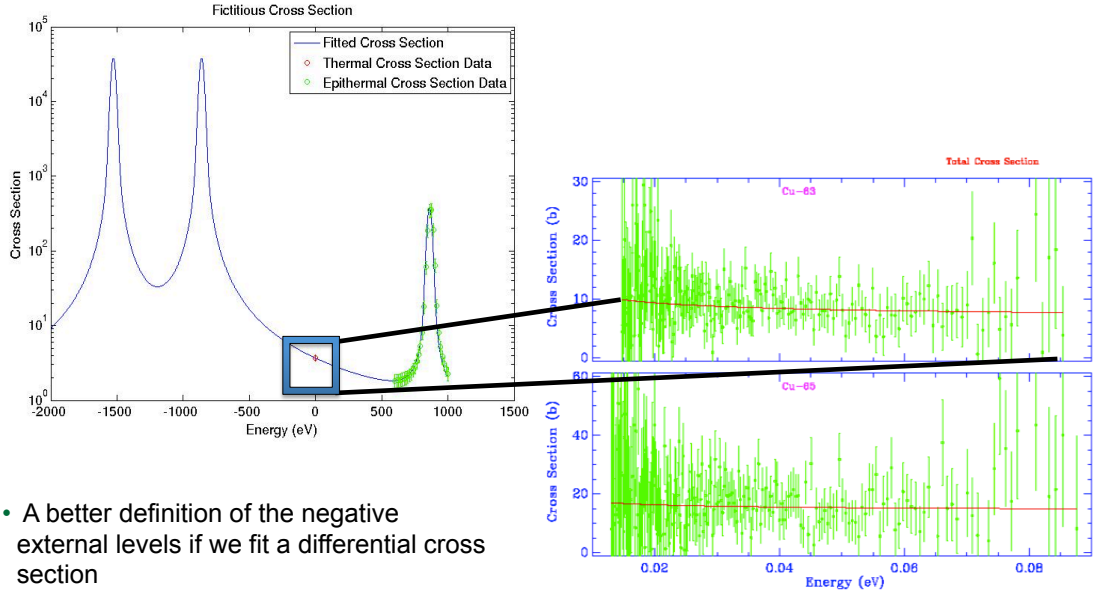
Total and capture cross section for ^{186}W in the energy range 500 eV to 1 keV



Cu Cross Section Evaluations (Sobes)

- **Motivation**
  - **Nuclear Data Advisory Group (NDAG) identified Cu-63 and Cu-65 as "IMPORTANT FOR MEASUREMENTS AND EVALUATIONS"**
  - **Purpose of Experiment:**
    - Thermal Cross Section Shape
    - Thermal Cross Section Uncertainty
    - SAMMY Resolved Resonance Analysis

Cu Cross-section Evaluations (Sobes)

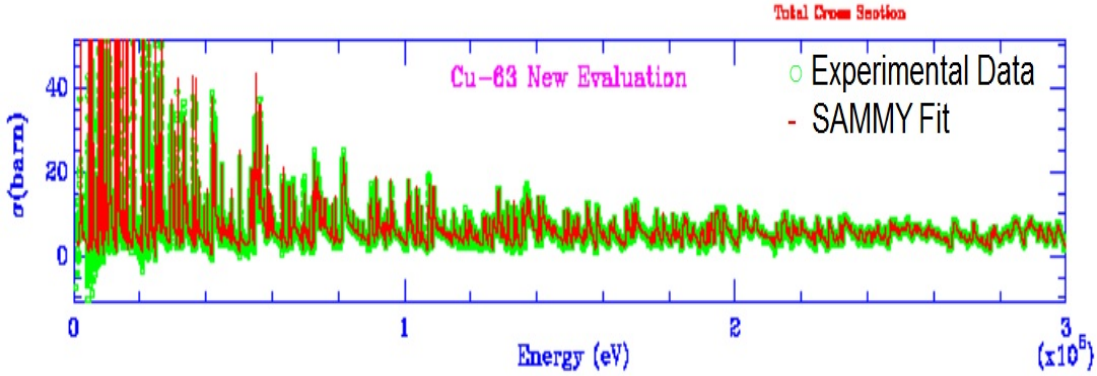


- A better definition of the negative external levels if we fit a differential cross section
- A better definition of the uncertainty and correlations at the thermal energy

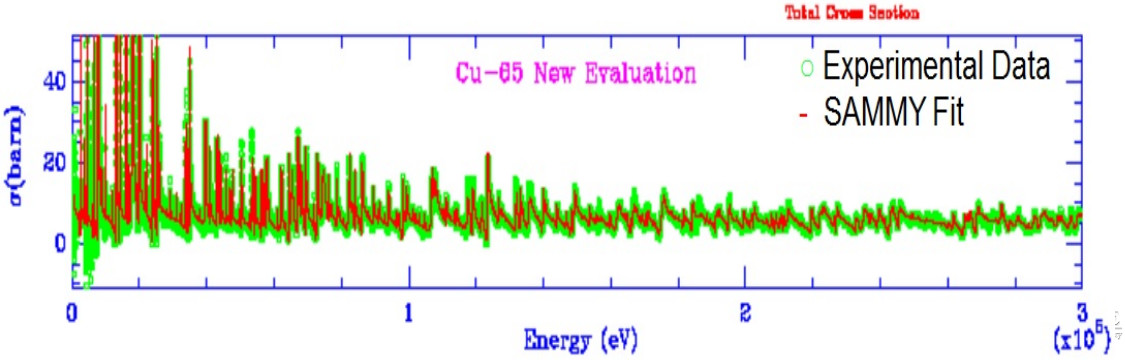
Cu Cross-section Evaluations (Sobes)

- **SAMMY Evaluation of the Transmission Data**
  - **SAMMY analysis of transmission data for Cu-63 and Cu-65**
  - **Measurements made at the Oak Ridge Electron Linear Accelerator (ORELA) by M. S. Pandey, J. B. Garg, and J. A. Harvey (1977)**
  - **Flight-path length: 80 meters**
  - **Thicknesses:**
    - Cu-63 0.07895 at/barns
    - Cu-65 0.07437 at/barns
  - **Energy Range: 0.0001 eV to 300 keV**

Cu cross section evaluations (Sobes)



SAMMY Fit of the transmission data of ^{63}Cu and ^{65}Cu in the energy range 30 eV–300 keV

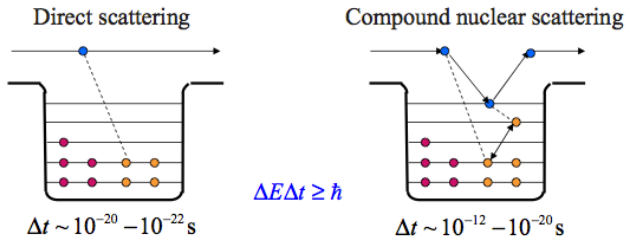


Cu Cross-section Evaluations (Sobes)

- Concluding Remarks
  - Measurement of thermal total cross sections at MIT was performed under the sponsorship of the (DOE) Nuclear Criticality Safety Program (NCSP)
  - Systematic and statistical uncertainties in the thermal region were determined
  - SAMMY analysis of the experimental data was performed for ^{63}Cu and ^{65}Cu in the thermal region
  - SAMMY analysis of the ORELA transmission data was performed for ^{63}Cu and ^{65}Cu
  - The present upper bound energy of the resolved resonance ENDF/B-VII.1 evaluations for ^{63}Cu and ^{65}Cu has been extended from 99 keV to 300 keV (paper accepted for presentation to PHYSOR 2012, Knoxville, TN)

APPENDIX: Formalities

- Direct and Compound nuclear scattering
  - At low energies, neutron-nucleus scattering occurs either directly or thorough the quasi-bound compound nucleus states
  - In a direct scattering, the incident neutron interacts with the average field of the nucleus. The duration of the collision is approximately the time it takes the neutron to cross the nucleus
  - In a compound nuclear scattering, the incident neutron loses energy upon colliding with the nucleus and is trapped. After a fairly long interval, enough energy is again concentrated on one neutron to allow it to escape.



APPENDIX: Formalities

All physical quantities can be defined by a set of resonance parameters

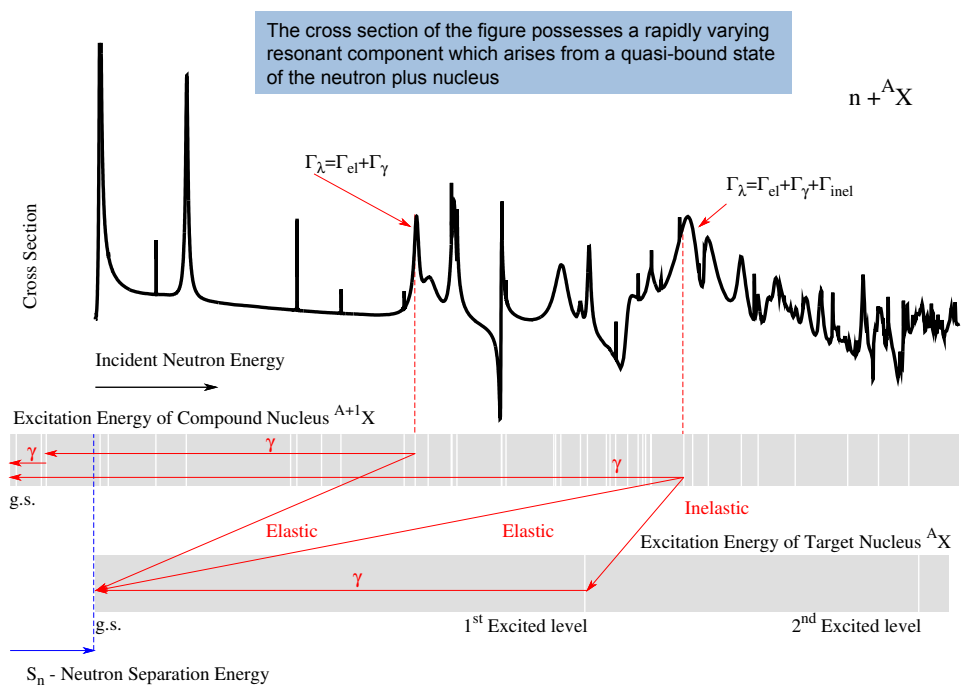
$$R_{cc'}(E) = \sum_{\lambda} \frac{\sqrt{\Gamma_{\lambda,c}}\sqrt{\Gamma_{\lambda,c'}}}{E_{\lambda} - E - i\Gamma_{\lambda,\gamma}/2}.$$

The relation between the scattering matrix and the R-matrix is

$$U_{cc'}(E) = \frac{I_l(k_c a_c)}{O_l(k_c a_c)} \frac{1 - R_{cc'}(L_l^* - B_l)}{1 - R_{cc'}(L_l - B_l)},$$

where I_l and O_l are the ingoing and outgoing radial wave-functions, respectively. Calculated for the channel radius a_c and wave number $k_c = \sqrt{2\mu_c E_c}/\hbar$. L_l and B_l are the logarithmic derivative of the outgoing and radial wave-functions.

The cross section for the entrance channel c and exit channel c' is given

$$\sigma_{cc'}(E) = \frac{\pi}{k_c^2} g_c \,|\, \delta_{cc'} - U_{cc'} \,|^2 .$$

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