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OVERVIEW OF THE U238 EVALUATION IN THE RESOLVED RESONANCE RANGE

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Motivation for a new evaluation of U238 resonances

- Evalution of U238 resonance parameters in ENDF\B-VI.8, JENDL3.3, JEFF3.0 by Moxon et al. In 1994 (0 -10 keV).
- Aim of the new evalution :
  - Include transmission measurements from J. Harvey et al. (ORELA, 1988, 1 keV – several hundred keV) and capture from Macklin et al. (ORELA, 1988)
  - Extension of the resolved range 10 keV ⇒ 20 keV
  - Investigate below 1 keV (thermal capture value, first large resonances, solid state effect...)
  - Improve (if possible) prediction of keff for thermal integral benchmarks. More information : see WPEC/Subgroup-22 and ueval@nea.fr forum

Status of U238 evaluation work

- Preliminary evaluation ORNL2 (0-20 keV) released last year for testing purpose : ueval@nea.fr .

- Improved evaluation ORNL3 presented at the Santa-Fe Conference ND2004 :
  - Analysis of Macklin et al. Capture data (1988)
  - Refined analysis of the range thermal - keV

- ORNL4 just completed and ready to be merged with LANL "high energy" evaluation and tested
  - Refined analysis of the range 1 keV – 10 keV

Experimental database

Energy Range	Reference	Measurement Type	Sample Thickness (at/b)	Flight path Length (m)
0.0253 eV	Poenitz et al. [9] ANL 1981	Activation		
Thermal Range	Corvi et al. [10] GELINA 1997	Capture	1 sample 0.0010	8.7
> 5 eV	Defilippo et al. [11] ORELA 1980	fission		40.
6 eV - 38 eV	Meister et al. [7] GELINA 1997	Transmission	4 samples U and UO_2	26.5
6 eV - 100 keV	de Saussure et al. [12] ORELA 1973	Capture	1 sample 0.0028	40.
0.5 eV - 4 keV	Olsen et al. [13] ORELA 1977	Transmission	7 samples 0.0002 to 0.175	42.
300 eV - 100 keV	Olsen et al. [14] ORELA 1979	Transmission	4 samples 0.0038 to 0.175	150.
250 eV - 130 keV .	Macklin et al. [4] ORELA 1988	Capture	2 samples 0.0031, 0.0124	150.
1 keV - 100 keV	Harvey et al. [3] ORELA 1988	Transmission	3 samples 0.0124 to 0.175	200.

Analyzed for the first time

Methodology

- SAMMY code, Reich Moore formalism
- Experimental parameters studied :
  - Norm, Background, Resolution, Cross Section Correction: Self-Shielding, Multiple Scattering, Doppler Broadening.
- Preliminary analysis for the determination of the best values for the experimental resolution function.
- Preliminary analysis for the determination of the External Resonance Parameters and of the Effective Scattering Radius R', (R' = 9.45 fm)

- In the energy range 0 eV to 20 keV:
  - 898 s-wave resonances D=22.3 eV
  - 849 p1/2 resonances D=23.6 eV
  - 1565 p3/2 resonances D=12.8 eV

3312 resonances

Resonance parameters below 103 eV

NSTD

Energy	Γ_γ meV present work	Γ_n meV present work	Γ_γ meV ENDF/B-VI	Γ_n meV ENDF/B-VI	Γ_n meV present work Γ_γ from ENDF/B-VI
	R' = 9.45 fm		R' = 9.42 fm		R' = 9.45 fm
6.674	23.01 ± 0.02	1.475 ± 0.001	23.00	1.493	1.476 ± 0.001
20.871	23.12 ± 0.03	10.04 ± 0.01	22.91	10.26	10.07 ± 0.01
36.682	23.41 ± 0.04	33.43 ± 0.02	22.89	34.13	33.55 ± 0.02
66.031	23.64 ± 0.10	24.17 ± 0.04	23.36	24.60	24.23 ± 0.03
80.747	23.31 ± 0.41	1.877 ± 0.01	23.00	1.865	1.877 ± 0.01
102.56	24.53 ± 0.14	70.62 ± 0.08	23.40	71.70	71.03 ± 0.08

Adopted in the present ORNL evaluation
Because it gives better results on integral exp.

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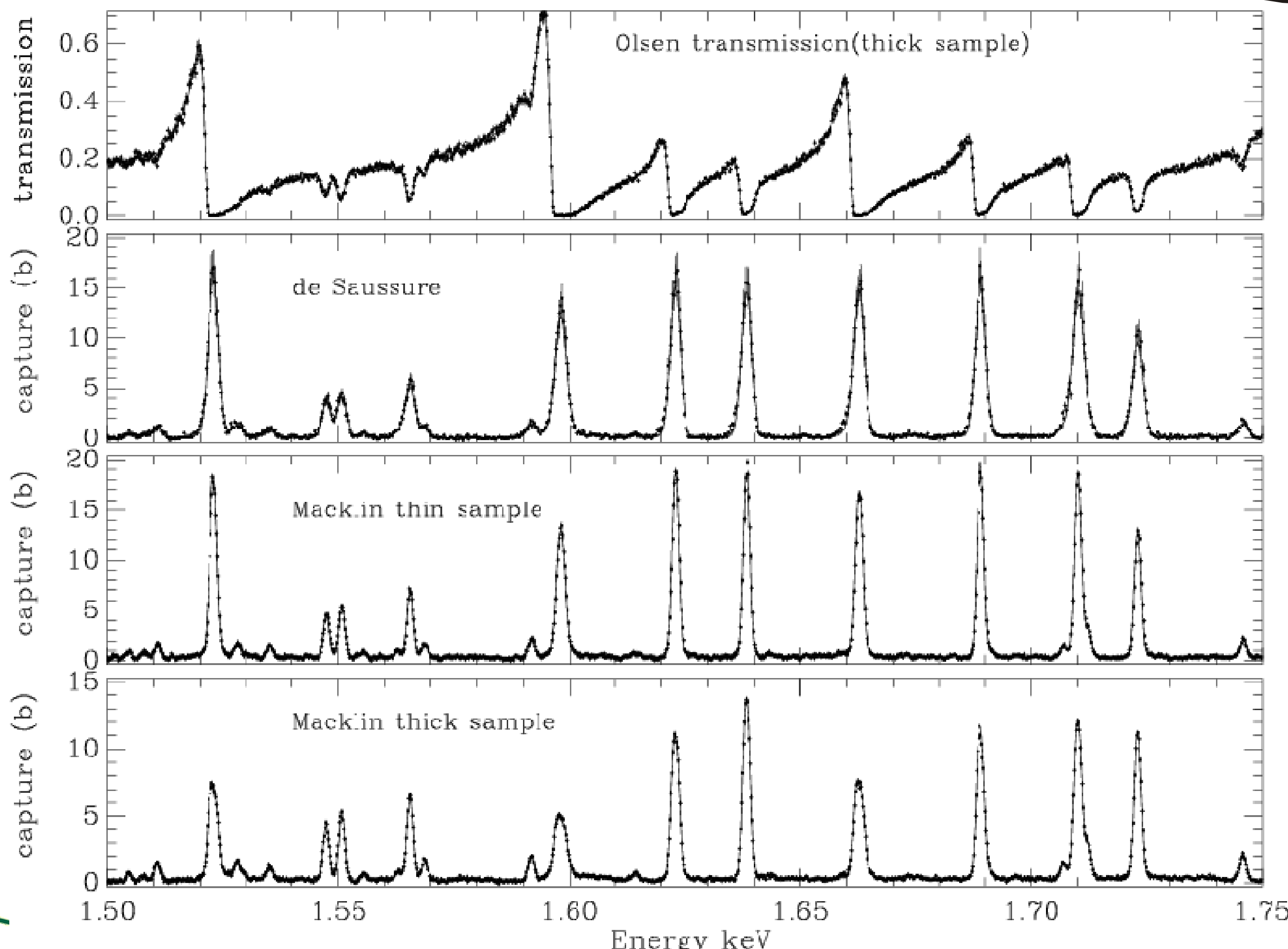
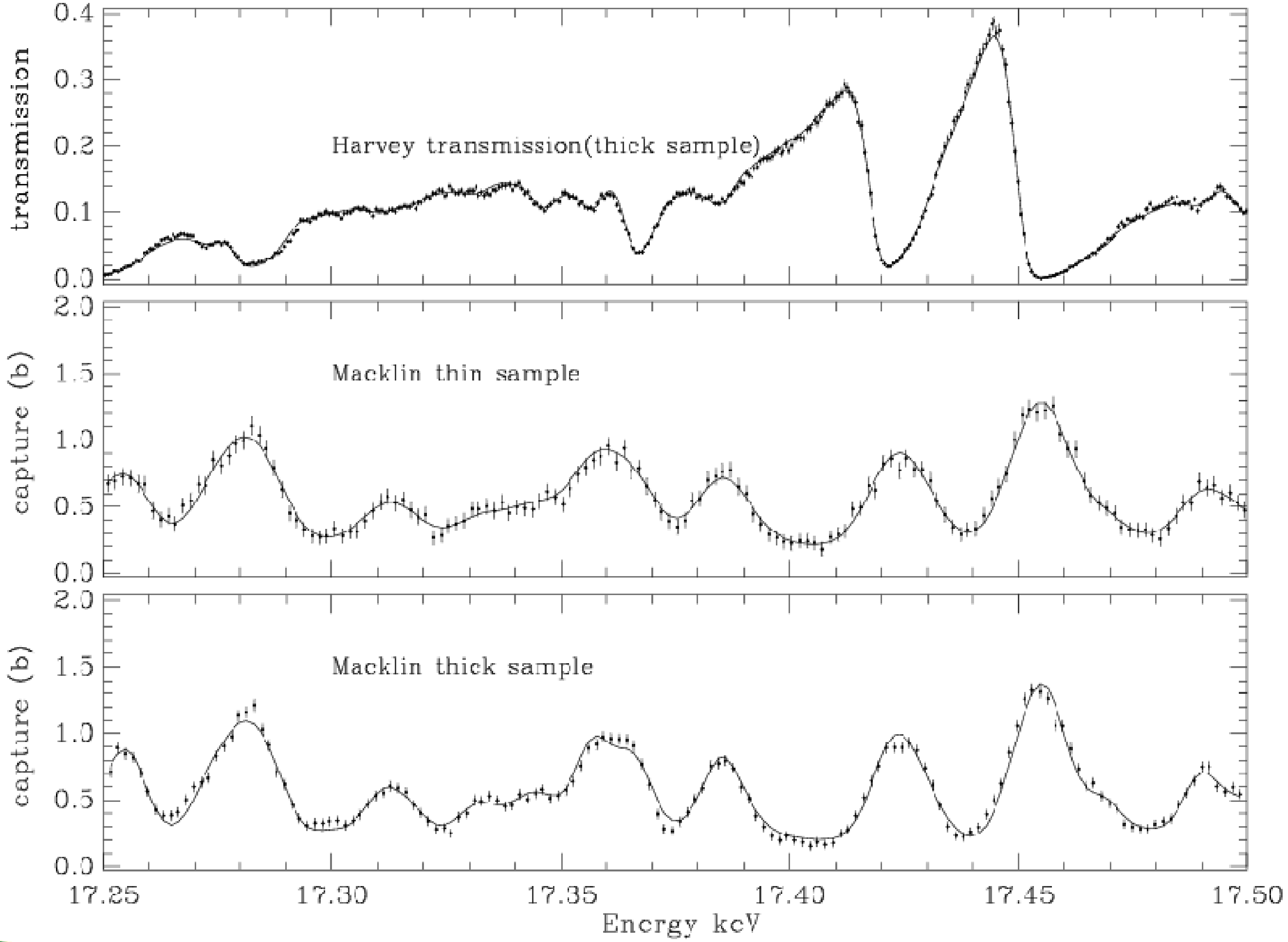
ornl

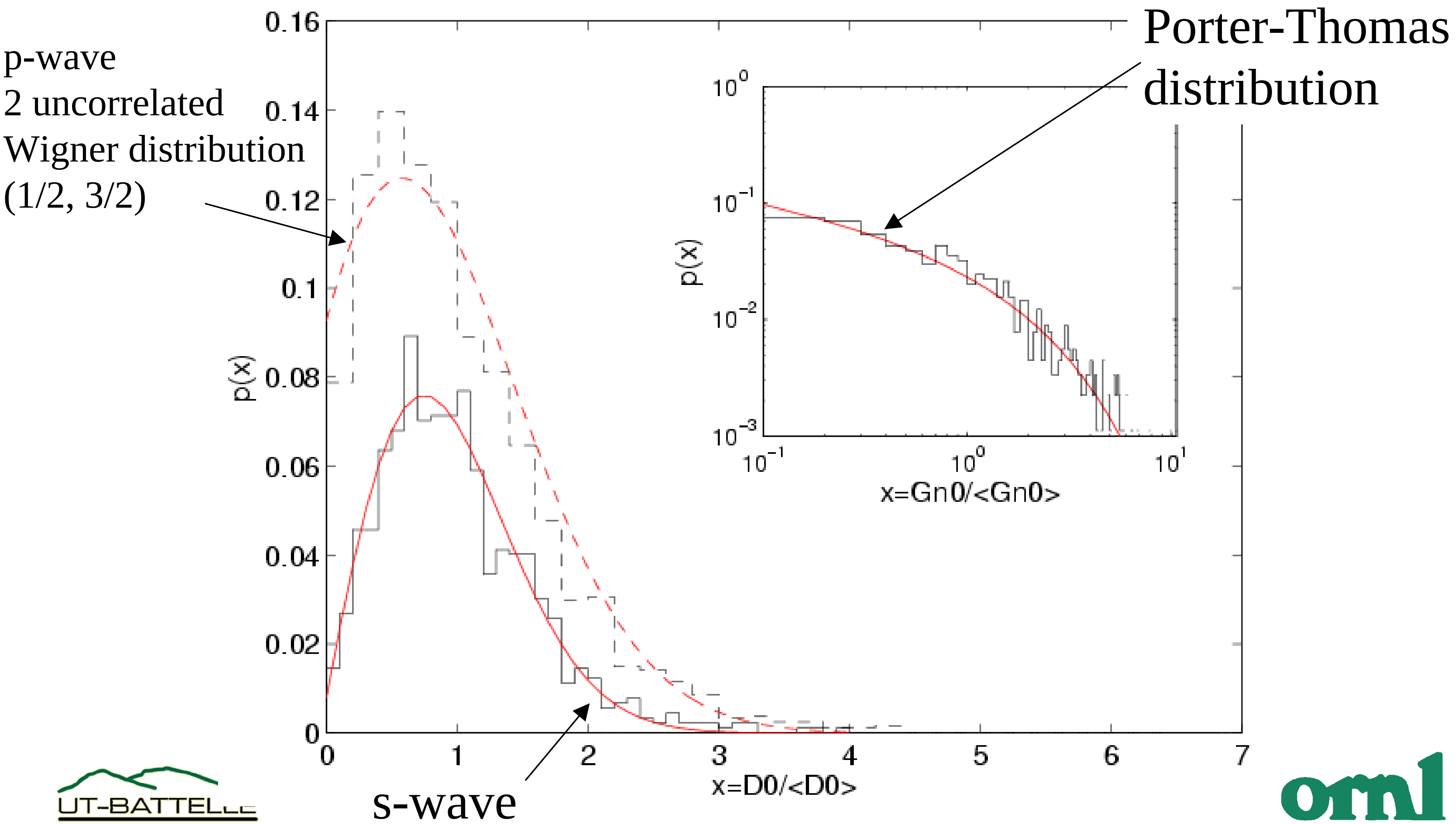
Exemple of fit : 1.5 – 1.75 keV region



Exemple of fit : 17.25 keV – 17.50 keV



Statistical properties of resonance parameters



Choice of thermal cross-section

- Thermal capture cross-section adjusted : $\sigma_0 = 2.683 \pm 0.012$ b following recent work of A. TrkoV
- Thermal scattering cross-section adjusted on bound coherent scattering length measurements :

Meas.	Value of b fm	4*pi*a2 b
Atoji et al. (1961)	**8.55 ± 0.06 fm**	**9.38**
Roof et al. (1962)	**8.4± 0.2 fm**	**9.06**
Willis et al. (1963)	**8.5 ± 0.06 fm**	**9.27**
Koestler (1974)	**8.63 ± 0.04 fm**	**9.56**
Mughabgahb	**8.55 ± 0.04 fm**	**9.38**
Boeuf et al. (1982)	**8.407 ± 0.007 fm**	**9.08**

a : free coherent length
b : bound coherent length, accurately measured by neutron interferometry

$$a = f(b)$$

Discrepant values

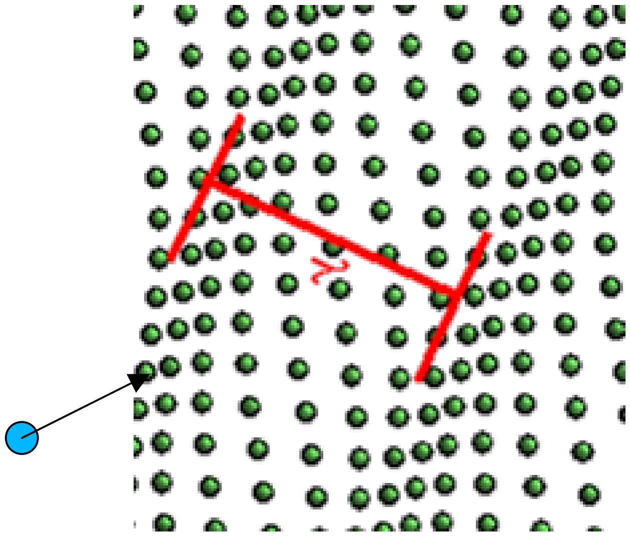
Not yet included in the evaluation

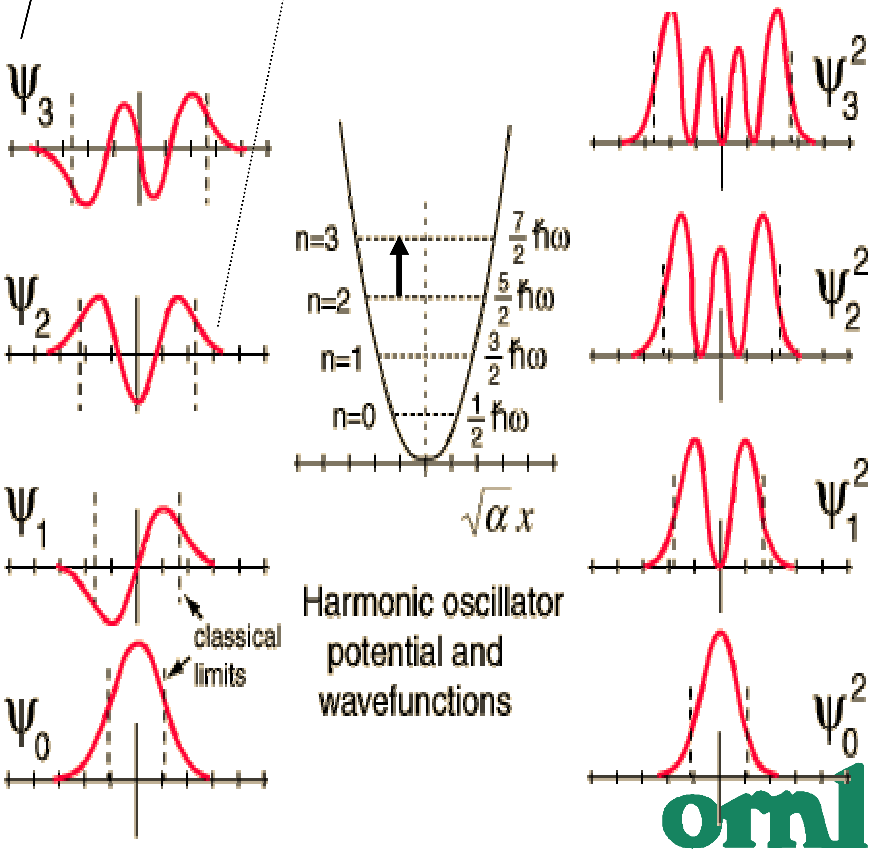
Solid state effect in Doppler broadening

- Resonance analysis usually based on Free Gas Model
- Effective temperature used to simulate solid state effects
  - Lamb's prescription (not valid for the first s-wave U238 resonances)
  - Temperature fitted
- More rigorous Crystal Lattice Model implemented in SAMMY recently by N. Larson (based on the DOPUSH code, D. Naberejnev et al.)

CLM theory (Lamb 1937)

$$\sigma_\gamma(E) \propto \Gamma_n \Gamma_\gamma \sum_{a,b} \frac{g(a)|<b\,|e^{i\vec{k}.\vec{r}}|a>|^2}{(E - E_0 + \varepsilon_a - \varepsilon_b)^2 + \Gamma^2/4}.$$





The Crystal Lattice Model

$$\sigma_\gamma(E) = \int_{-\infty}^{\infty} S(\vec{k}, E')\sigma_\gamma^{T=0}(E - E')dE'$$

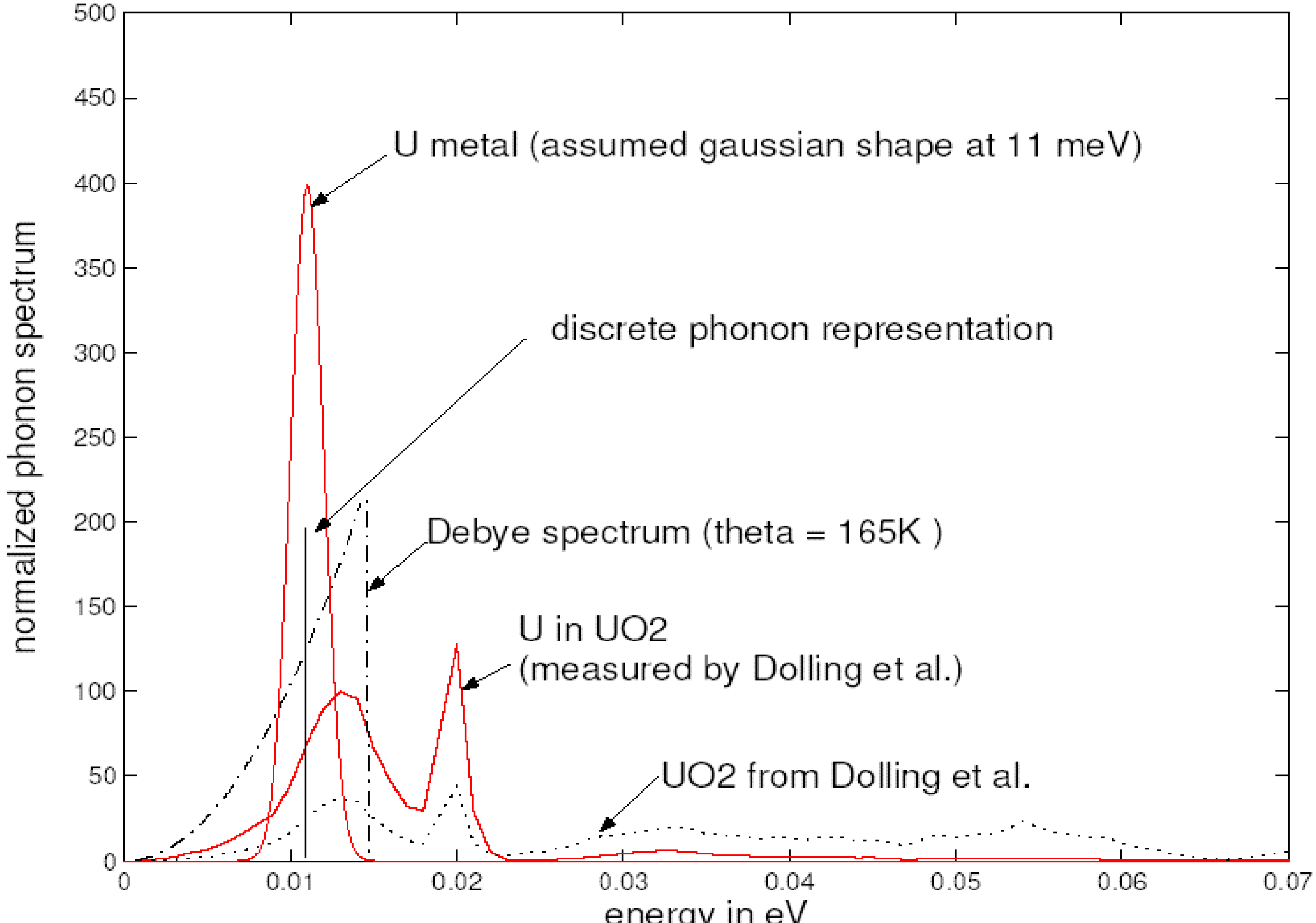
With

$$S(E,E') = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iE't} e^{\frac{mE}{M+m}[\gamma(t)-\gamma(0)]} dt \qquad (5)$$

and

$$\gamma(t) = \int_0^{+\infty} \frac{\rho(\hbar\omega)}{\hbar\omega}[coth(\frac{\hbar\omega}{2kT})cos(\omega t) + isin(\omega t)]d\hbar\omega.$$

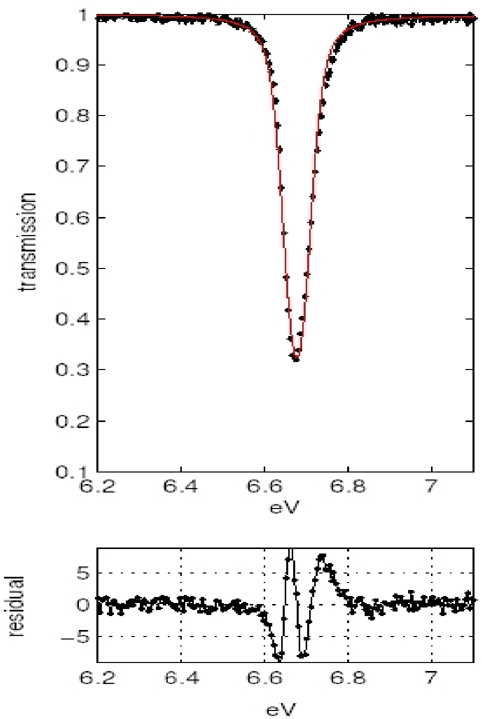
Uranium metal and oxide phonon spectrum



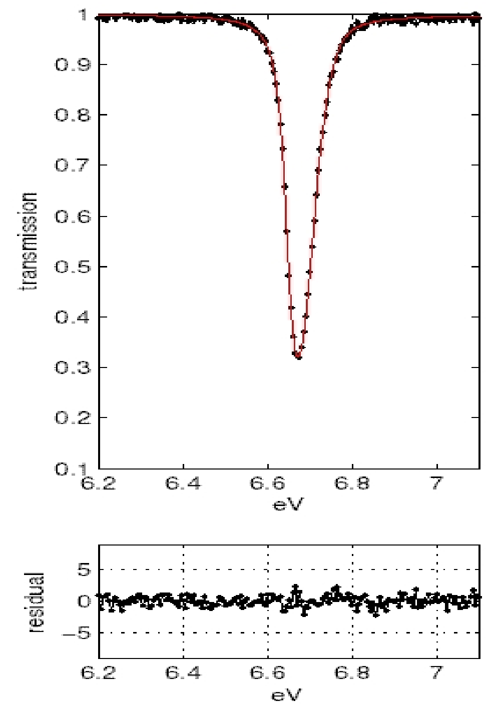
U238 fit with the Free Gas Model (FGM) and Crystal Lattice Model (CLM) of SAMMY

→ test of SAMMY-CLM on U238 transmission (GEEL) at low and room temperature (Meister 1997)

Ex :
UO2
thick sample
23.7K



FGM + adjT



CLM with Dolling et al. Phonon spectrum

Olsen et al. Measurements (1977) 6.67 eV resonance (u-metal 300K)

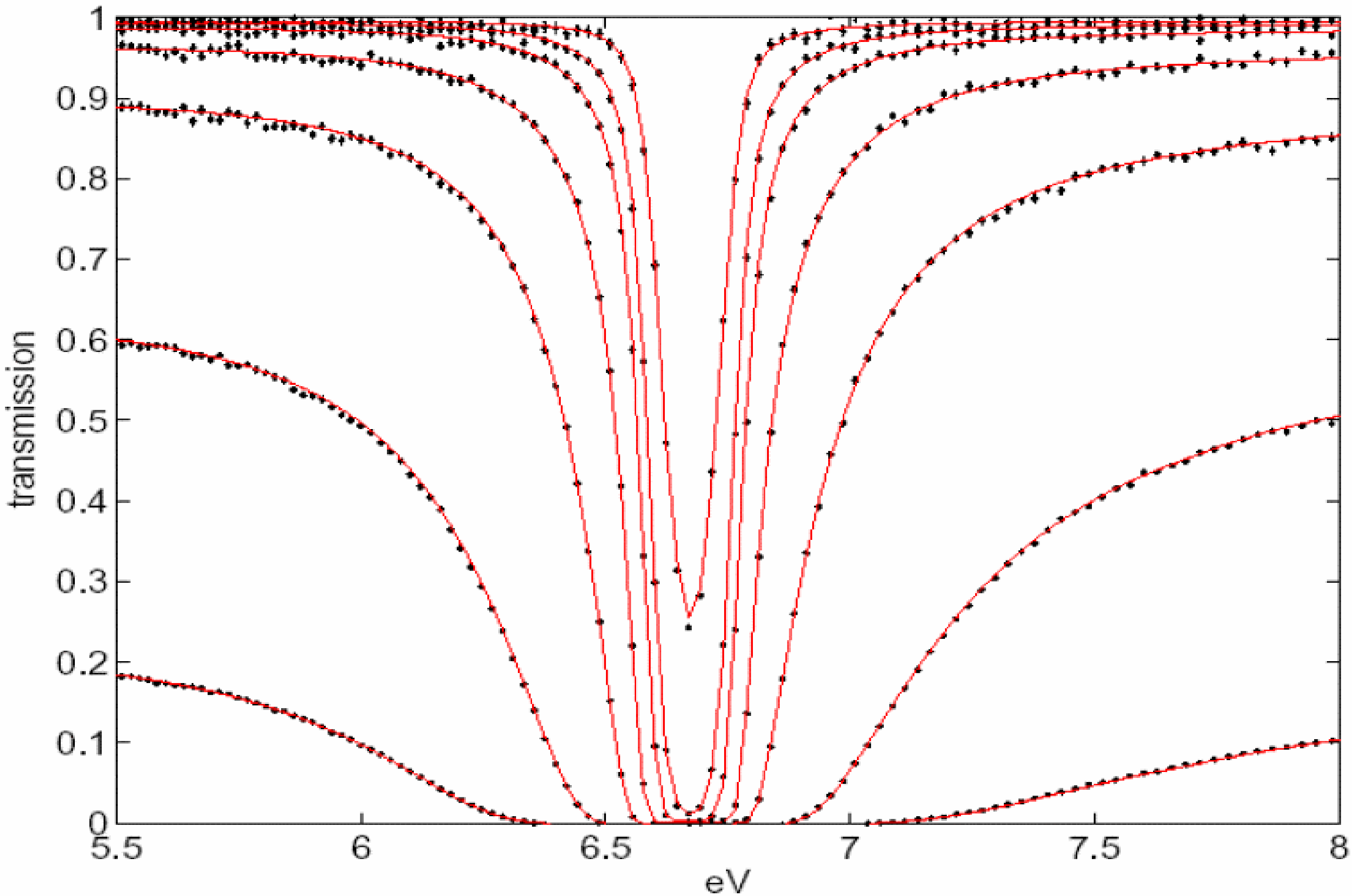


TABLE 3. Comparison of FGM versus CLM resonance parameters of the 6.7 eV resonance from sequential fits of Olsen et al. [12] transmission data. Uncertainty values take into account only statistical errors and are strongly underestimated.

Method	E_r eV	Γ_γ meV	Γ_n meV
$R' = 9.45 fm$			
FGM $T = 300$ K	6.6742	23.09	1.471
FGM $T_{fit} = 296.8$ K	6.6741	23.08	1.473
CLM $T = 293$ K	6.6734	23.02	1.476
Statistical uncertainty	0.0001	0.02	0.001

Conclusion on solid state effect

- **CLM of SAMMY improves fits on U238 low temperature measurements**
- **Small impact on U238 extracted resonance parameters for room-temperature, u-metal measurements**

Advantage

- **Choice of temperature**

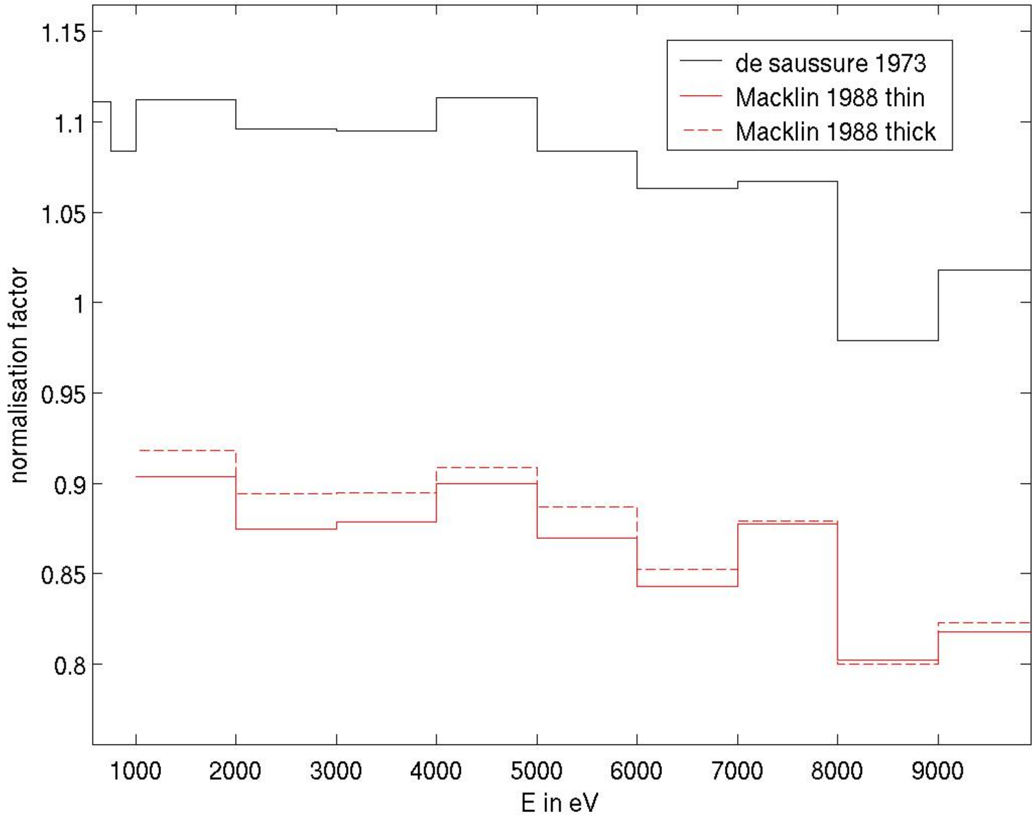
Drawback

- **Computation time**

Phonon spectrum needs to be known

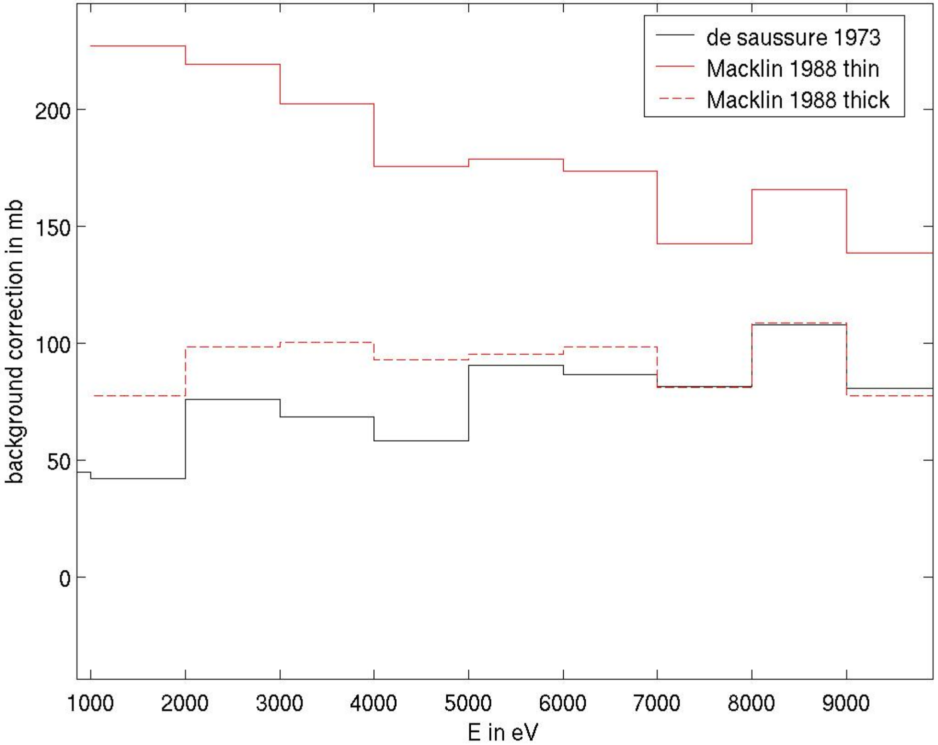
Accuracy of U238 capture cross-section measurements

Normalization factor obtained from the SAMMY fit



Direct capture at thermal and low energy for U238 ?

Background values obtained from the Sammy fits of Capture measurements



- Mughbghab estimates 80 mb at thermal energy (Lane-Lynn formalism)
- uncertainties on spectroscopic factors measured by (d,p) reaction

Direct capture at thermal and low energy for U238 ?

Theoretical estimate (see ND2004 paper by Arbanas et al.)

Direct-Semidirect Neutron Capture Calculations Applied to R-Matrix Data Evaluations in the Resolved Resonance Region

G. Arbanas*, F. S. Dietrich† and A. K. Kerman**

TABLE 1. Summary of thermal capture results and comparison with prior works; all cross sections listed in mb; a systematic error of ±20% comes mostly from the uncertainty in the measurements of the spectroscopic factors

Author	^{19}F	^{27}Al	^{28}Si	^{29}Si	^{30}Si	^{35}Cl	^{37}Cl	^{39}K	^{41}K
This work *	6.5	60	133	111	98	430	418	799	544
Rauscher†	—	—	65	58	67	160	310	—	—
Raman-Lynn**	4.6	—	134	116	100	—	—	—	—
Lane-Lynn ‡	4.7	108	107	70	64	—	400	753	1,320
Exp.	9.5	231	169	119	107	43,600 §	433	2,100	1,460

* A real part of the Koning-Delaroche OMP [11] was used for DSD.
† Performed with TEDCA program; direct capture only.
** based on R-matrix theory with complex OMP and valence capture
‡ Taken from Mughabghab [12], based on Lane and Lynn [2].
§ Thermal capture dominated by a nearby compound resonance

Interference in the capture channels ?

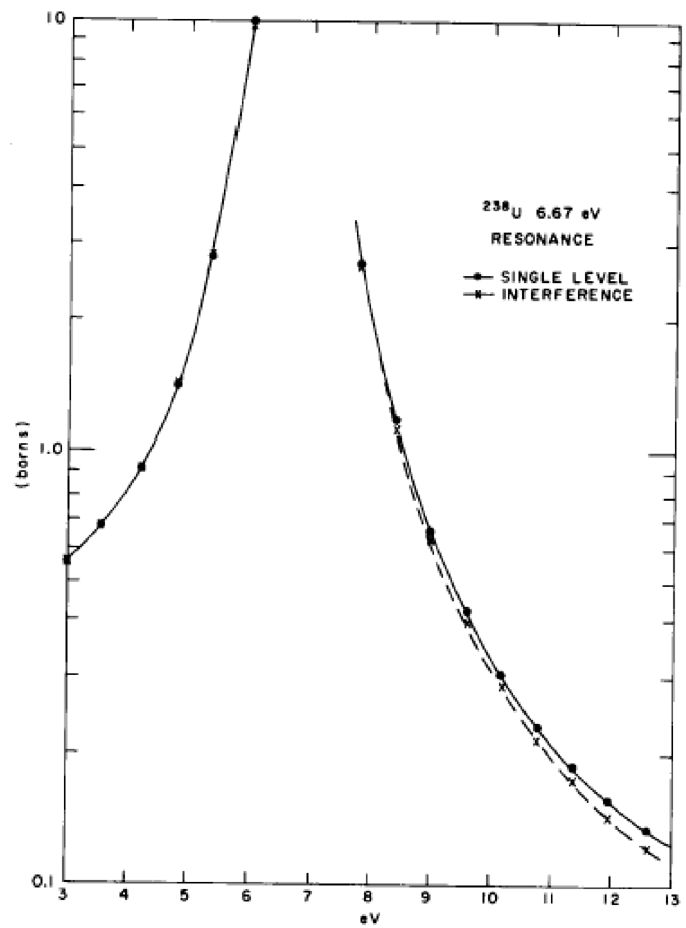
- Evaluation based on Reich-Moore Formalism
  - Large number of exit channel in capture
  - off-diagonal radiation widths average to zero (radiative widths amplitude have randoms signs)

- But in U239, one transition (4059 keV to ½- state) has a higher probability (~10% of the total capture)

- Might cause asymmetry in the capture resonance shape (interference effect)

Interference in the capture channels ?

R. E. Chrien (1975)
Seminar on U238 capture
6.7 eV resonance



Integral testing

- ORNL2 + LANL high energy extensively tested
  - Good results on thermal benchmarks (LCT)
- ORNL4 + new-LANL just started (Bob Mc Farlane, MCNP)
  - Still good results on thermal benchmarks

Work in progress

- "cosmetic changes" in the resonance parameters file
  - Thermal scattering cross-section value
  - Class-II resonances
  - No impact on integral results

- U238 unresolved range (20 keV – 150 or 300 keV) , new features :
  - Analysis of Macklin capture data (1988 – ORELA) and Harvey transmission data (1988 – ORELA) in the range 20 – 100 keV

Conclusion

- **Evaluation of U238 resonance parameter "ORNL4" completed**
- **The new file is being merged with the LANL new "high energy" evaluation of Young et al.**
- **Should be available for integral testing soon.**