DE LA RECHERCHE À L'INDUSTRIE

NAUSICAA COLLABORATION:
FROM EXPERIMENTS TO NUCLEAR APPLICATIONS

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10-11 May 2016

NAUSICAA project

https://www.ill.eu/instruments-support/computing-for-science/data-analysis/nausicaa/

Nausicaa

Nausicaa collaboration

The NAUSICAA (**N**eutron **AU**gmented **S**αβ **I**n **C**ross sections **A**lternative **A**ssessment) project is a collaborative research study including the ILL, the IRSN, the CEA, the TUM, the ESS, the University of Florence and the Ecole Polytechnique de Montréal. This project started mid-2014, and aims at improving the accuracy of the international neutron cross section libraries for reactor physics by introducing direct measurements. The most direct consequence of this project will be the tremendous improvement heavy water reactors and cold sources modelling. This project is organized under the auspices of the OECD/NEA, which will bring us a strong support, and in collaboration with the IAEA.

One caveat of the neutron cross section libraries is indeed the evaluation process of thermal neutron cross sections in liquids, especially in hydrogenated liquids in which inaccurate approximations are employed. This problem could be solved by the direct use of measured structure factors S(Q,ω), where Q is the neutron momentum transfer and ω is the neutron energy transfer. Until now all evaluations related to thermal neutron were based upon experiments performed with a momentum transfer Q=0, like IR or Raman. The extension on the whole Q domain is carried out by approximate laws which become clearly wrong in the case of liquids like water. This means that measurements of a real S(Q,ω) enable to get rid of the extension laws approximations and thus to significantly enhance the accuracy of the cross sections.

The first step of the study is now completed. A paper has been submitted for light and heavy water and a detailed report has been published in the framework of the CRISP project. We have demonstrated the feasibility and the reliability of this method. Two additional steps are foreseen in the next future and will be carried out in parallel. One is the acquisition and refinement of accurate data on light and heavy water in several conditions of temperature and pressure, from ambient to supercritical conditions. The other is the study of cryogenic liquids like liquid hydrogen and deuterium, which will require several years to carry out the measurements in the best conditions.

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Next meeting ILL, Grenoble ⇒ 21-22 June 2016

NAUSICAA project

Experimental programs

2010

⇒ Light and heavy water in IN5 and IN4 at ILL **in cold operating conditions**

- H20: 285 K, 290 K, 294 K, 300 K 302 K, 311 K, 323 K (P = 1bar)
- D20: 250 K (ice), 295 K, 296 K, 325 K

2015

⇒ Light and heavy water in IN5 and IN4 at ILL **in hot operating conditions**

- T = 300 - 540 K and P=1 - 600 bar

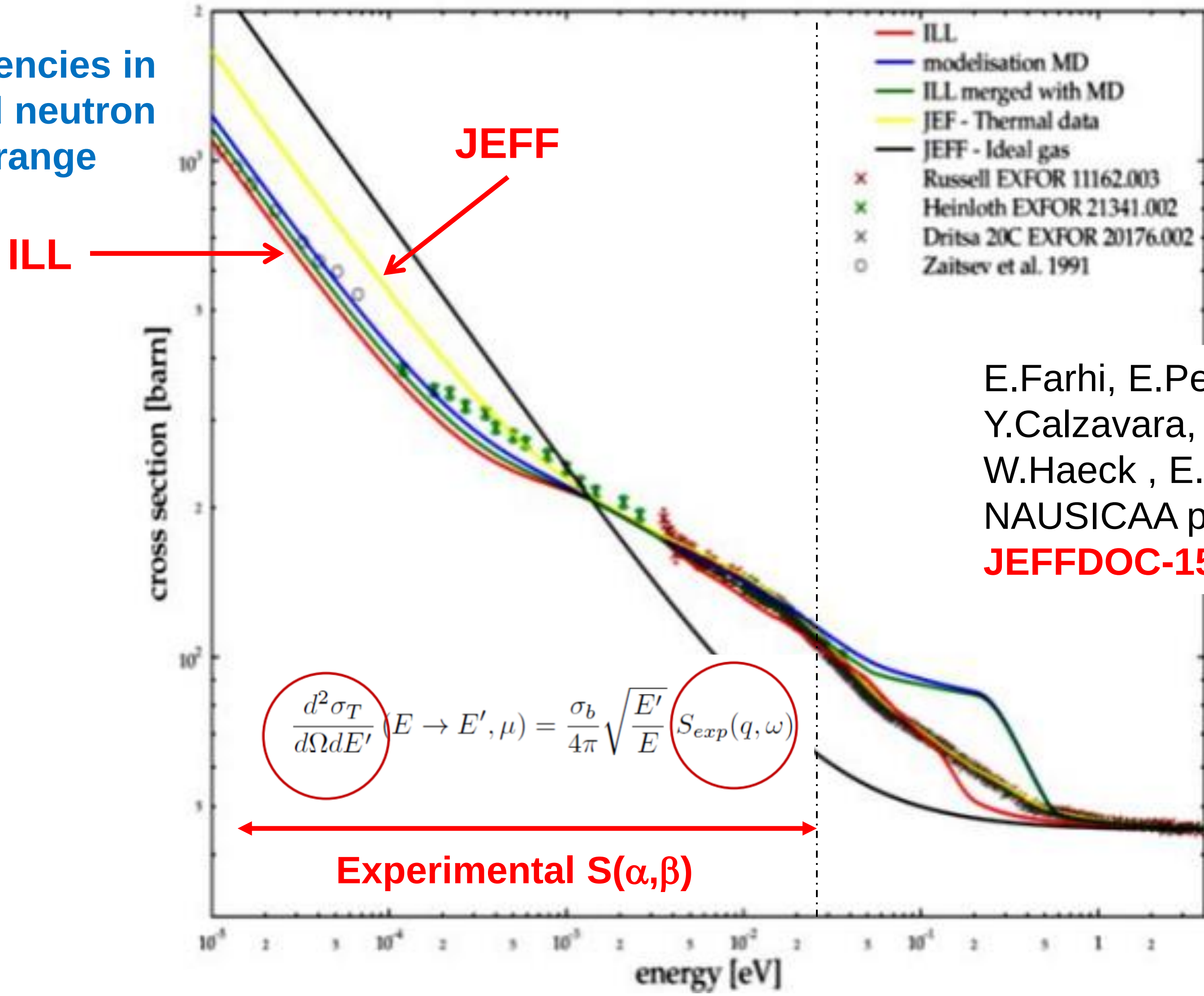
2016

⇒ Measurement of the double-differential neutron cross section of U in UO2 from room temperature to Hot Full Power conditions

Experimental program 2010 (H_2O, D_2O)

Large discrepencies in the cold neutron energy range

T= 300 K

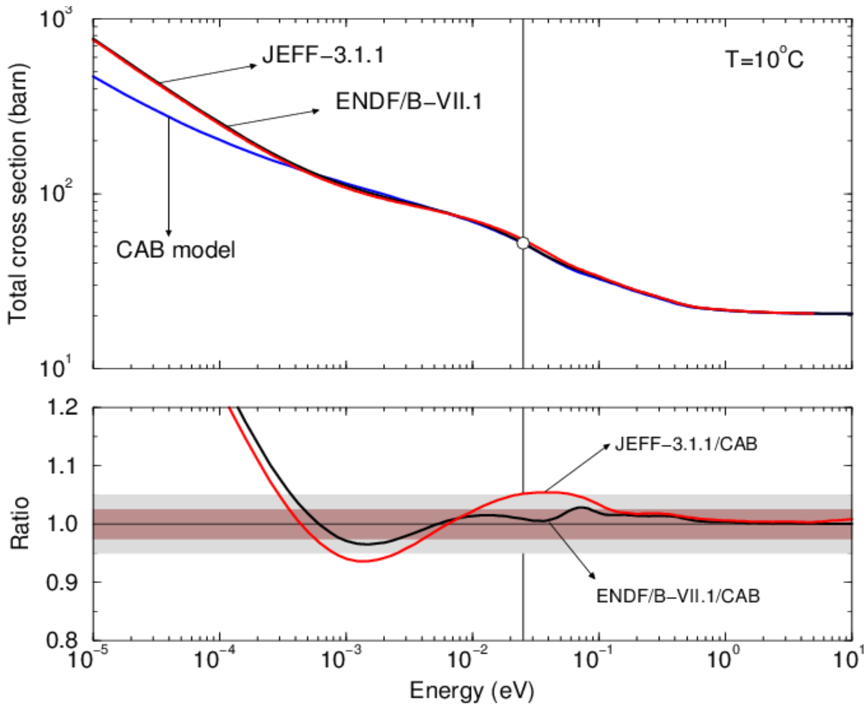


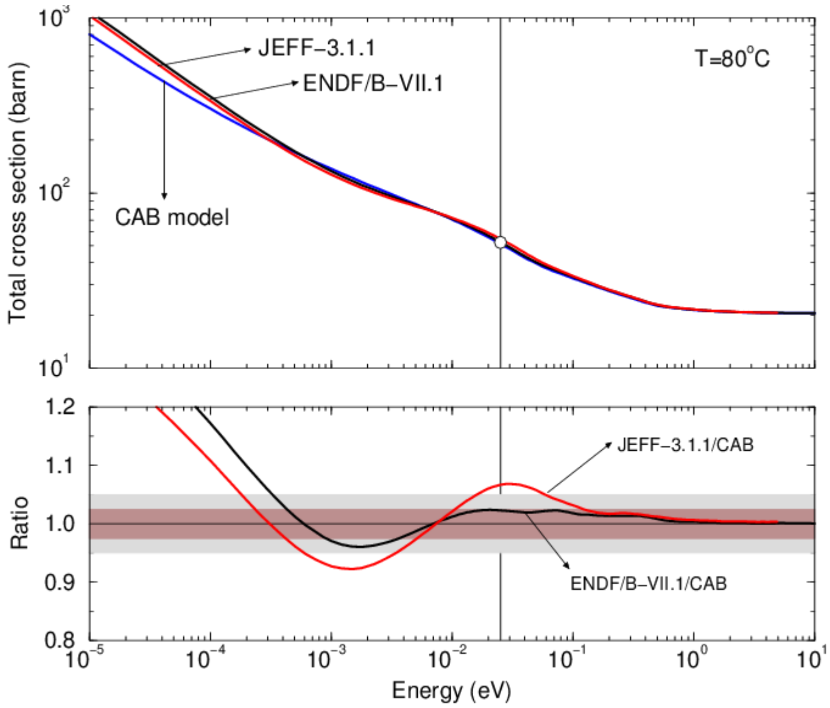
$$\frac{d^2\sigma_T}{d\Omega dE'}(E \rightarrow E', \mu) = \frac{\sigma_b}{4\pi}\sqrt{\frac{E'}{E}}\, S_{exp}(q, \omega)$$

E.Farhi, E.Pellegrini, Y.Calzavara, G.Ferran, W.Haeck , E.Guarini, NAUSICAA project, **JEFFDOC-1578**

Experimental program 2010 (H2O, D2O)

The sizeable discrepancies below the thermal energy are confirmed by the CAB model





Experimental program 2010 (H2O, D2O)

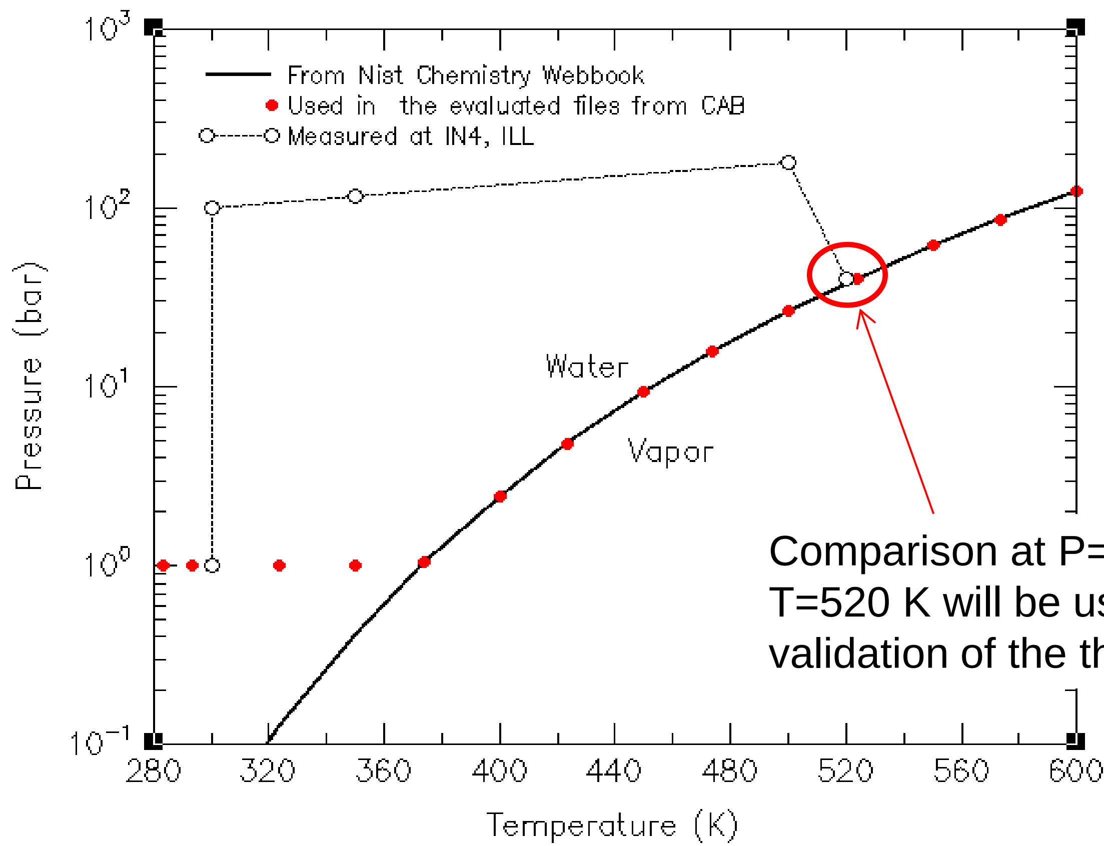
References

- Ghislain Ferrand, “Nouvelles méthodes numériques pour le traitement des sections efficaces nucléaires », PhD Thesis, 2014

- E. Farhi, G. Ferran, W. Haeck, E. Pellegrini and Y. Calzavara, "Light and heavy water dynamic structure factor for neutron transport codes", *J.Nucl. Sci. Tech*. 52 (2015) 844

Experimental program 2015 (H2O, D2O)

Comparison of the experimental conditions investigated at ILL and available in the ENDF files generated at CAB.

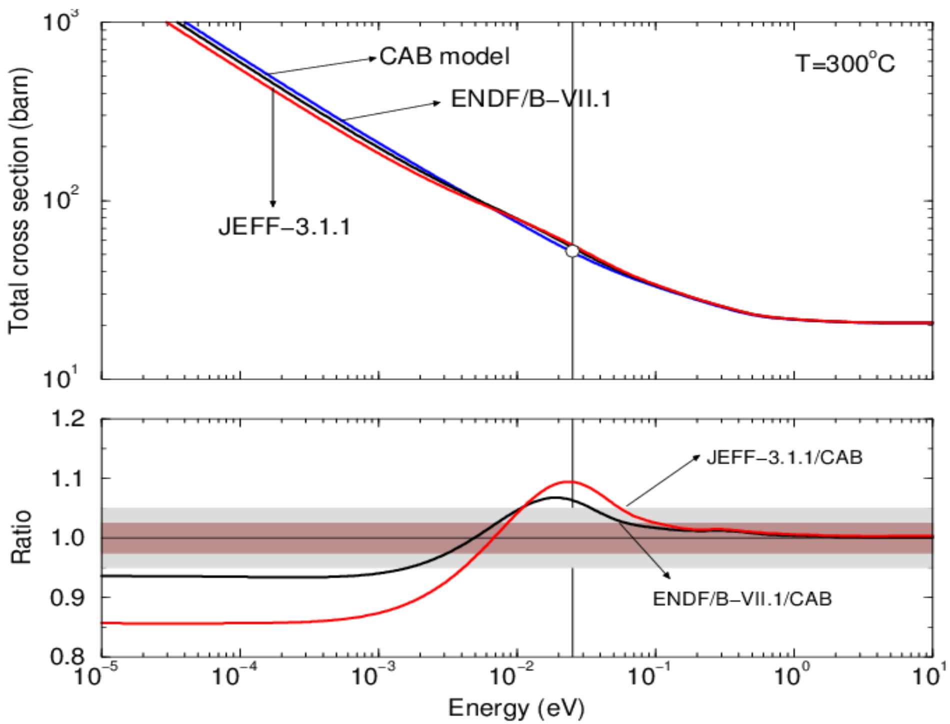


Comparison at P=40 bar and T=520 K will be useful for the validation of the theoretical model.

Experimental program 2015 (H2O, D2O)

Preliminary results obtained in Hot Zero Power and Hot Full Power conditions with JEFF-3.1.1 and CAB model

Benchmarks	T	H(H2O)	Δ
Configuration HFP	600 K	C(JEFF-3.1.1)-C(CAB model)	-10 pcm
Configuration HZP		C(JEFF-3.1.1)-C(CAB model)	-10 pcm



Good agreement between JEFF-3.1.1 (Mattes, 2005) and CAB model has to be confirmed !

⬇

Comparison with ILL data is needed

⬇

See presentations of V. Jaiswal, J.P. Scotta and E. Farhi

Experimental program 2016 (UO2)

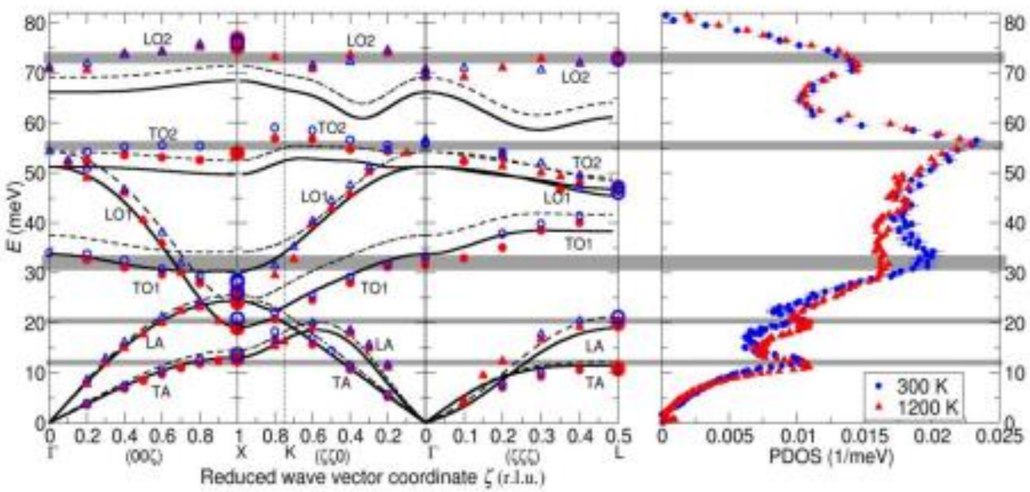
⇒ Problem was adressed by Danila Roubstov (kick off meeting, 18-19 May 2015)

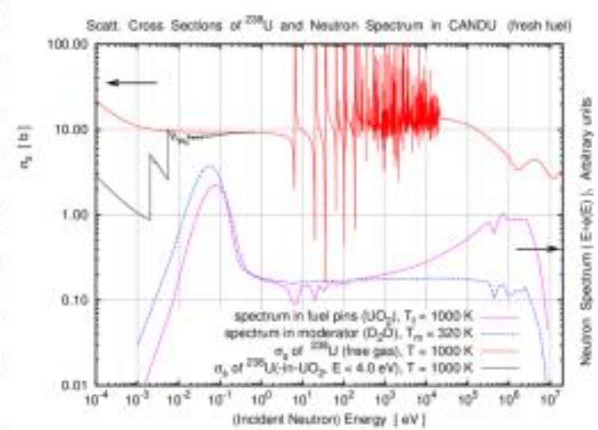
TSL for UO_2: phonon PDOS + coh. elastic

Phonons in actinides: active area of research,

Judy Pang *et al.*, Phonon density of states and anharmonicity of UO_2 ,

PHYSICAL REVIEW B 89, 115132 (2014)



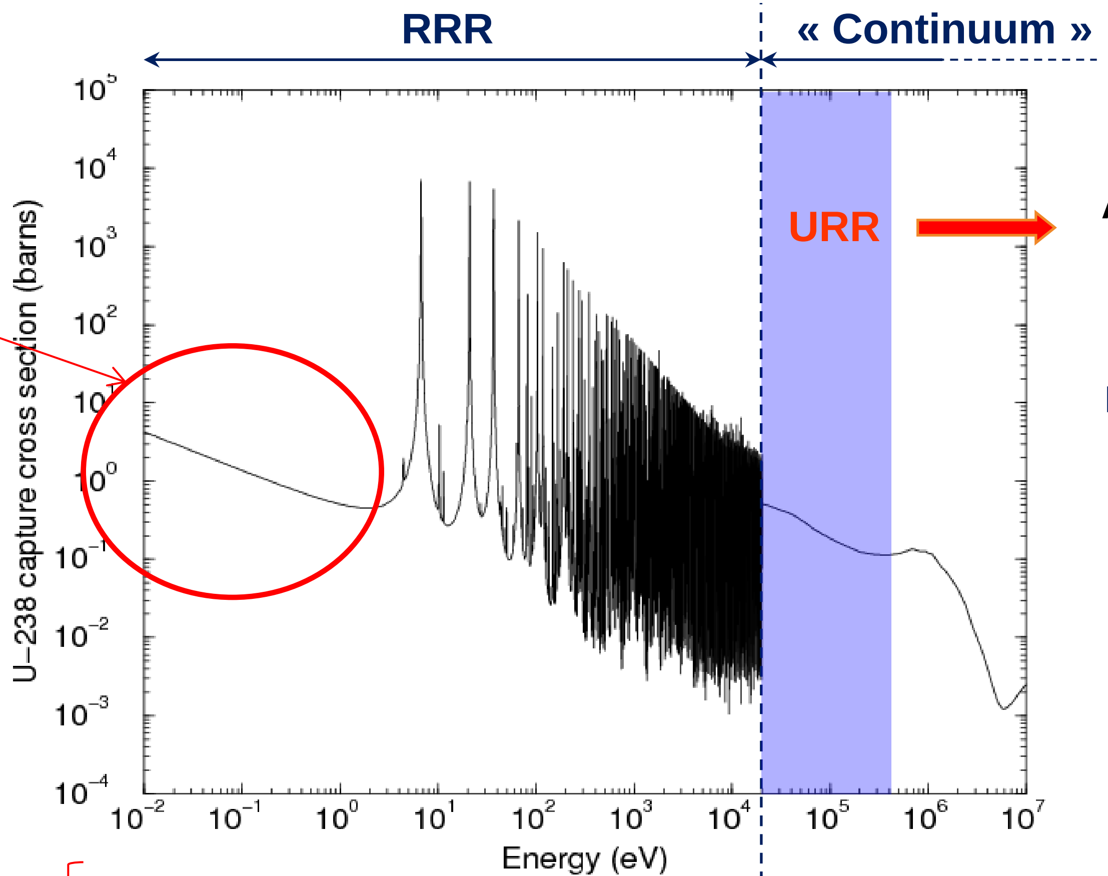


In reactor physics, for safety and licensing application:

fuel temperature coefficient of reactivity (FTC); T can go ~ 2000 K

Nuclear reaction models for U238

LEAPR model
of the
NJOY code



Average R-Matrix parameters

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Probability Tables

R-Matrix formalism

Optical model (ECIS)

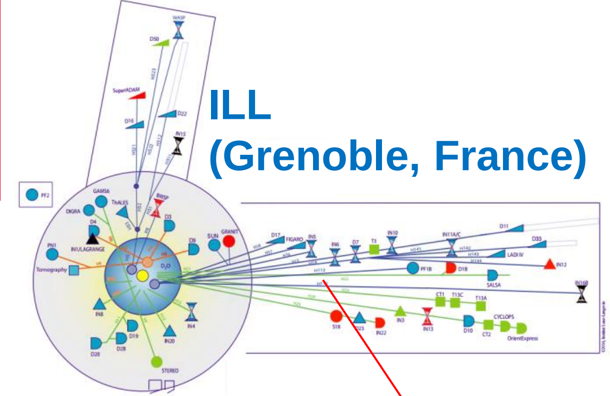
Statistical model (TALYS)

Conrad

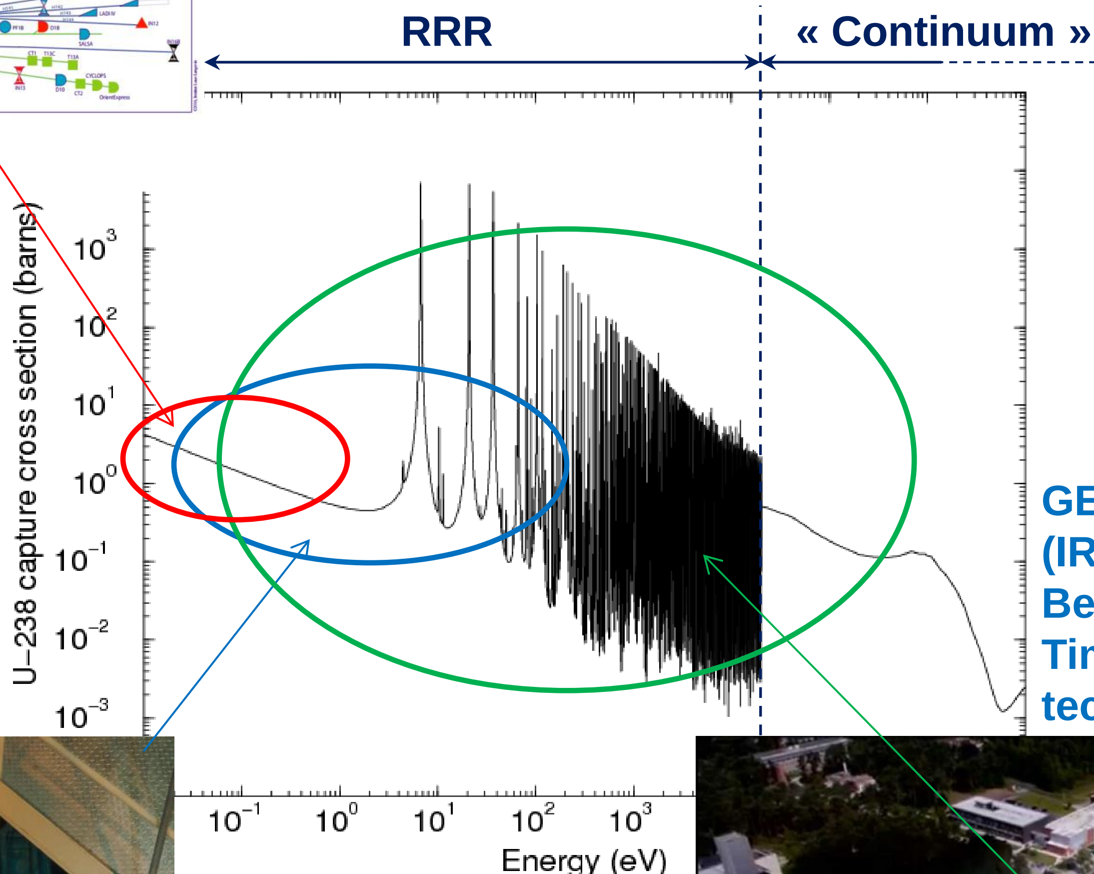
méthode ESTIMA

méthode SPRT

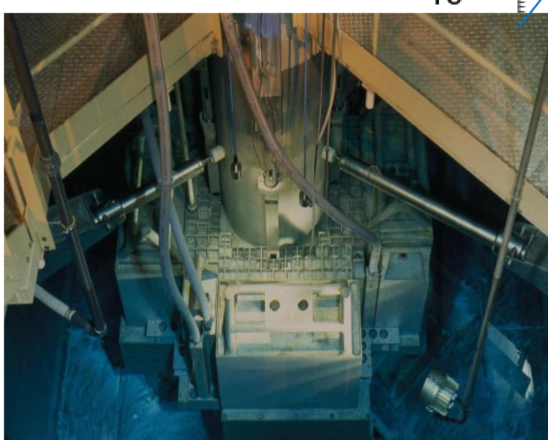
Experimental facilities



ILL
(Grenoble, France)

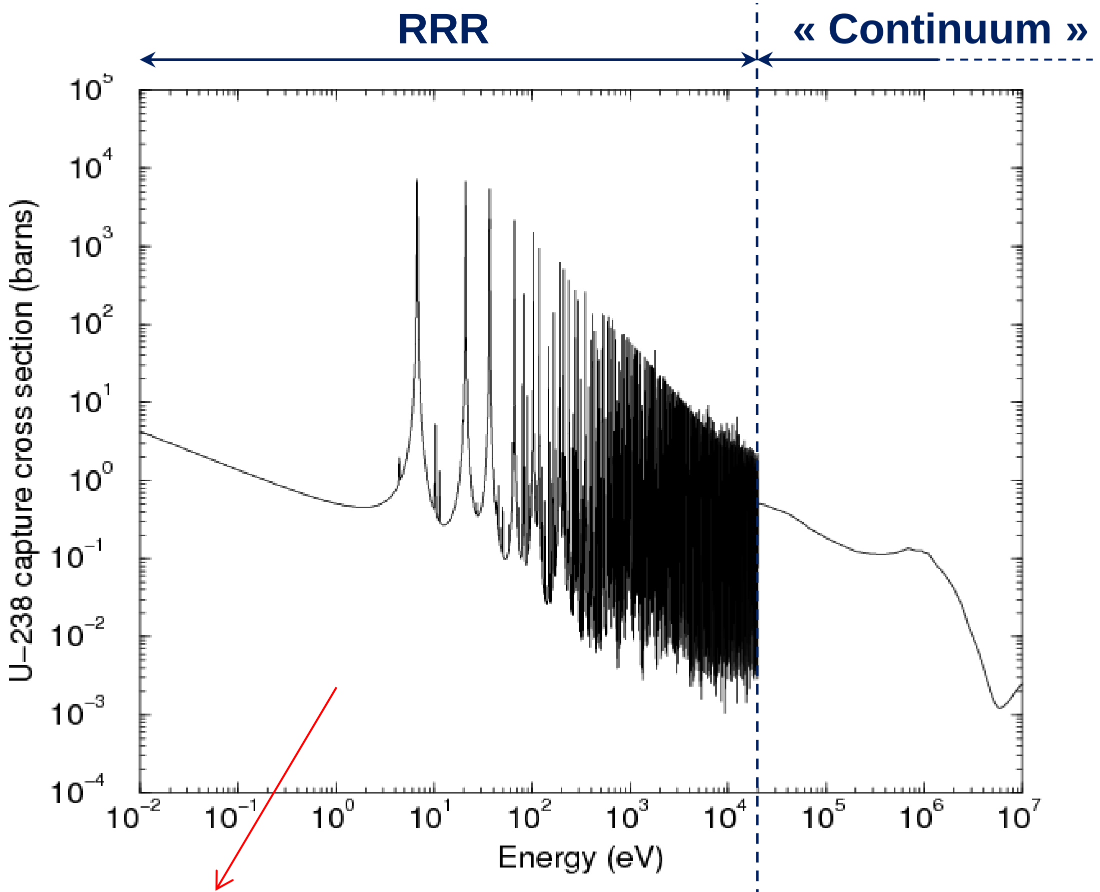


GELINA facility
(IRMM, Geel, Belgique)
Time Of Flight technique



MINERVE reactor
(CEA, cadarache)
Oscillation and activation measurements

Temperature dependent effects



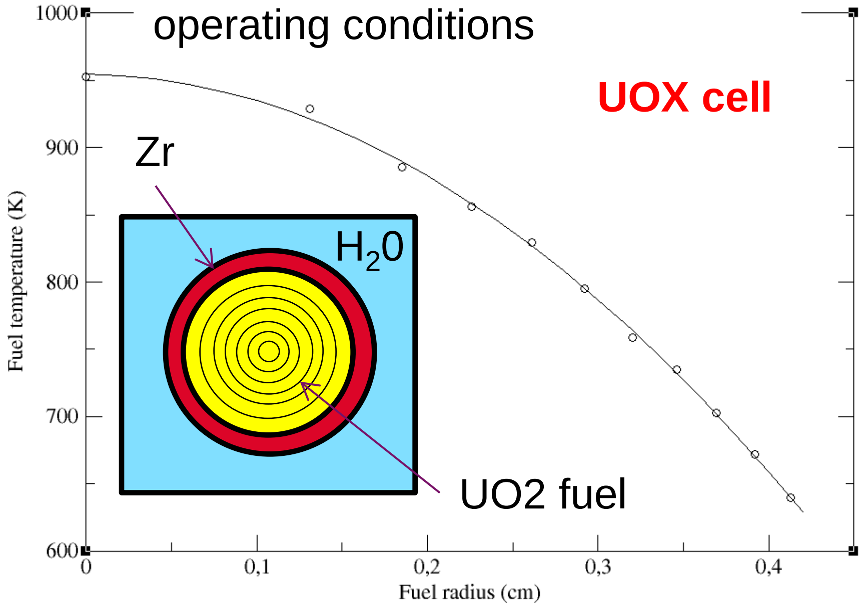
Temperature dependent effects of interest for nuclear applications

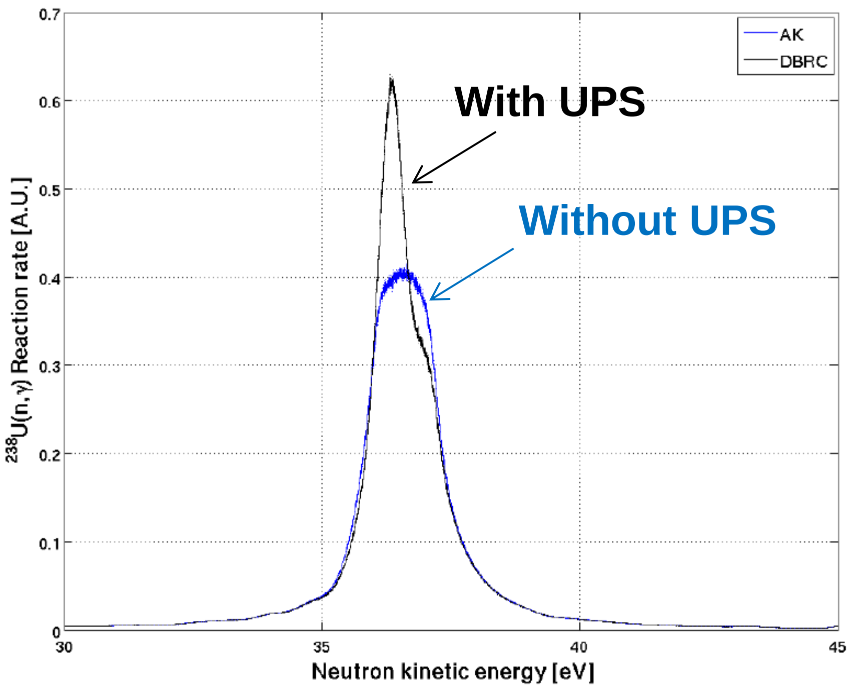
Cristal lattice and Ups-scattering effects

⇒ No microscopic data at high temperature (T>300 K)

Reaction rate calculated in a UOX cell with TRIPOLI4

Example of “temperature profile” inside the fuel pellet in hot operating conditions





UPS accounts for the thermal motion of the target nucleus in the energy transfert probability during the lifetime of the compound nucleus

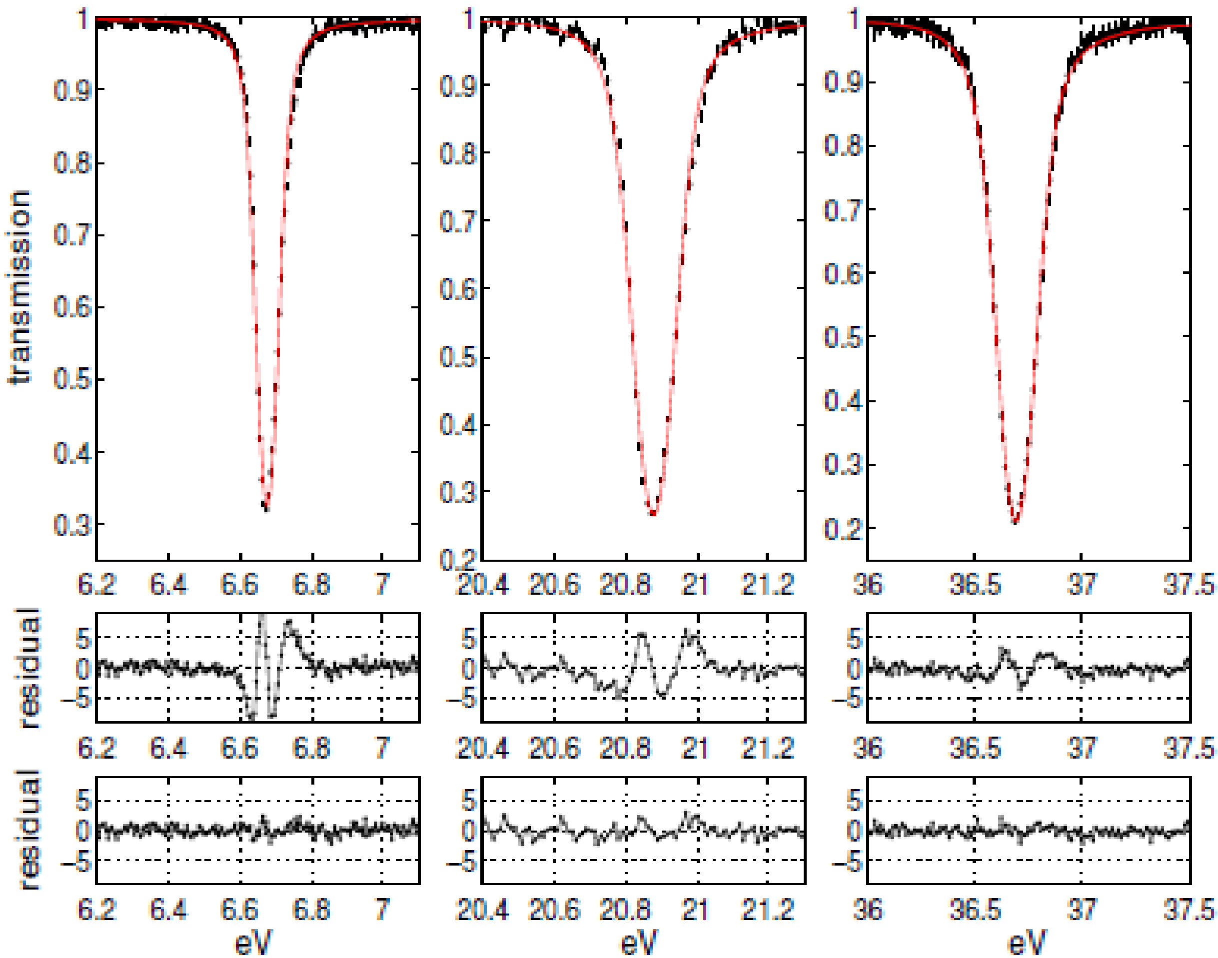
Sizeable impact at high temperature : at T=1000 K ⇒ -300 pcm on the calculated reactivity

Capture of neutrons by atoms in a crystal lattice T=77K

UO2 data measured at the GELINA facility (see ND2004)
SAMMY calculations with the Dolling's spectrum

Transmisison
UO2 sample

T=77 K



With FGM

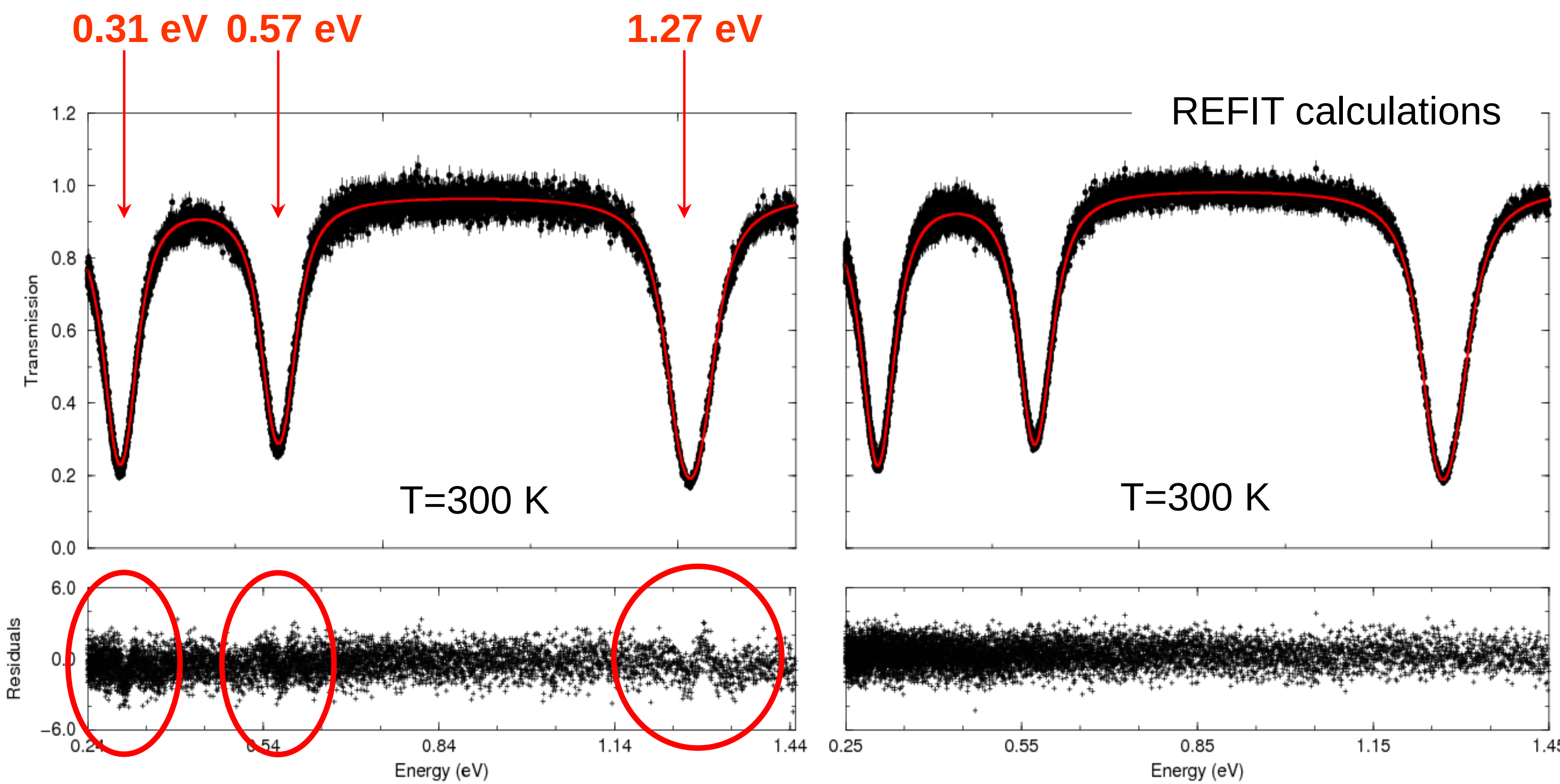
With CLM

⇒ Sizeable impact at low temperature

Capture of neutrons by atoms in a crystal lattice T=300K

Similar results are observed on Am241 at room temperature

C. Lampoudis et al. Eur. Phys. J. Plus, 128, 86 (2013)

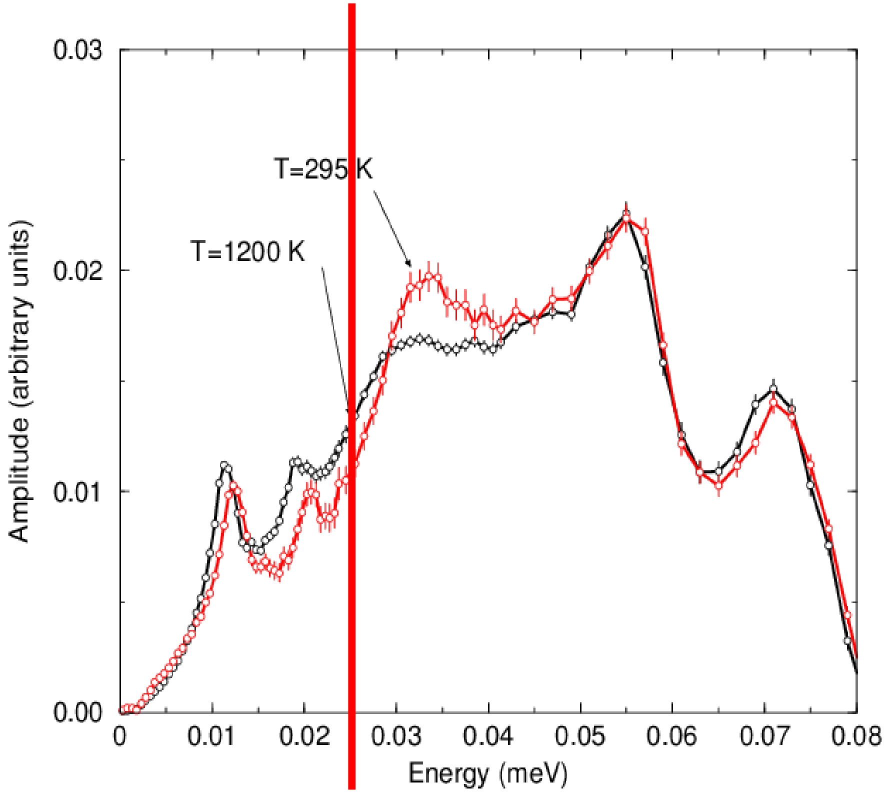


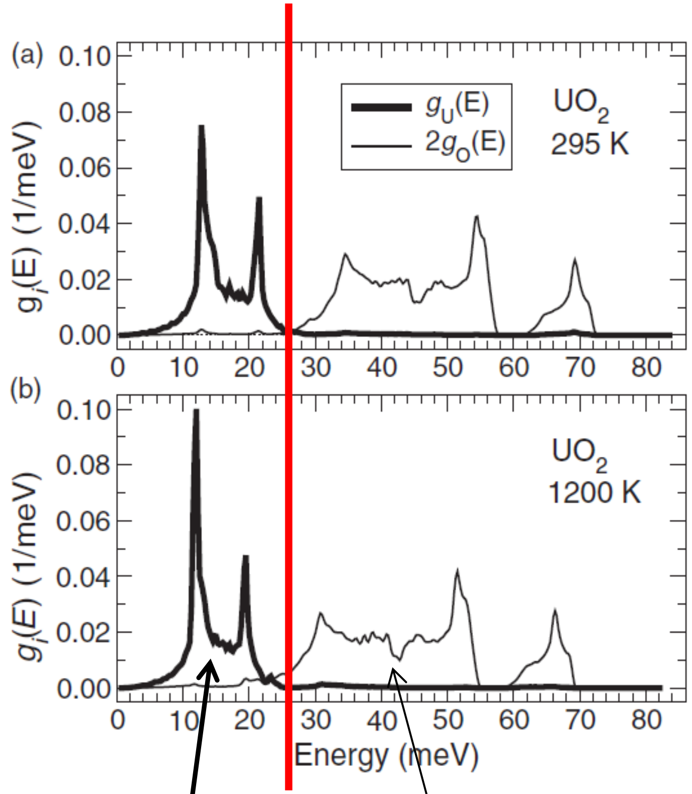
Free Gas Model (FGM)
with an effective temperature

Cristal Latice Model (CLM)
with the Dolling's phonon spectrum

Phonon spectrum

New experimental results from Pang et al. (Phys. Rev. B 89, 115132, 2014)

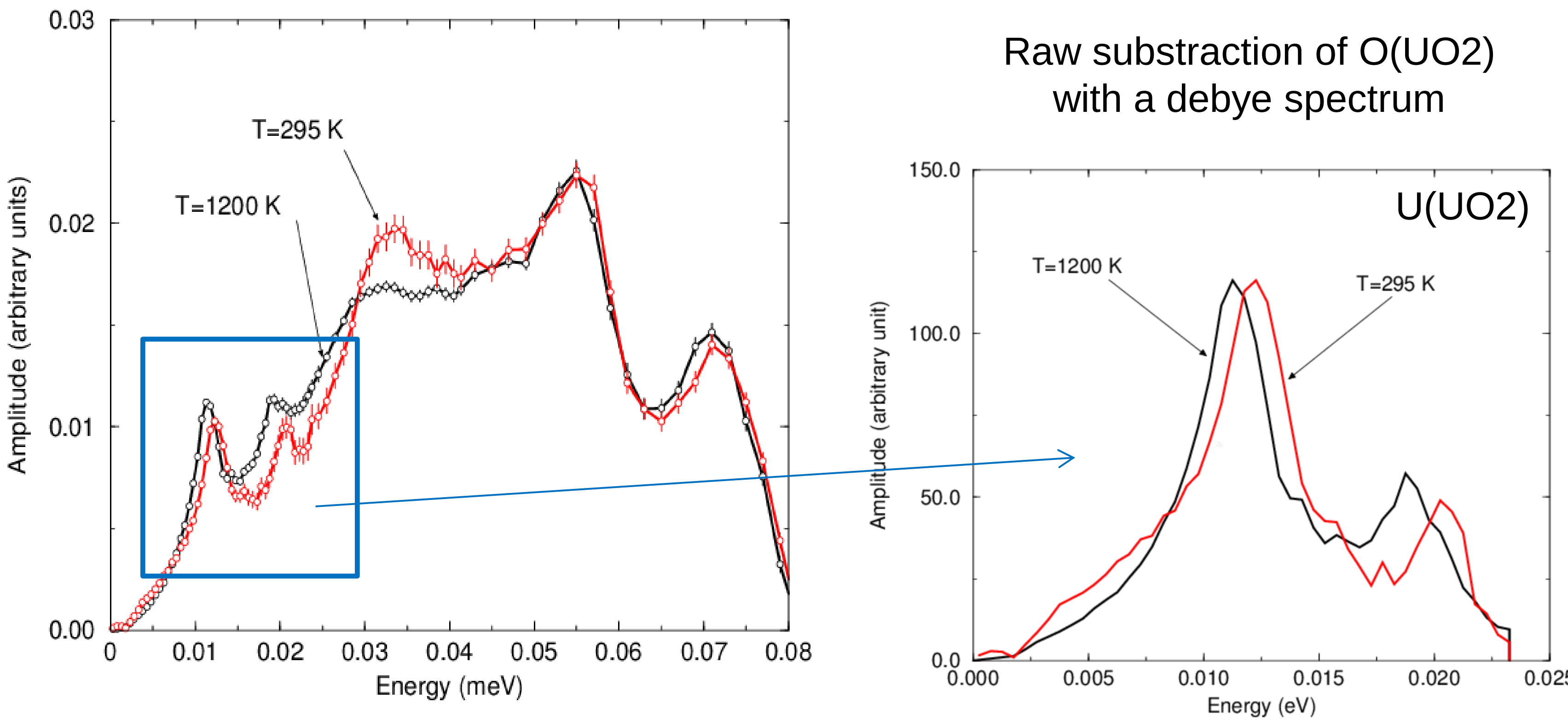




ab initio calculations show a clear separation of the **U(UO2)** and O(UO2) contributions

Phonon spectrum

New experimental results from Pang et al. (Phys. Rev. B 89, 115132, 2014)

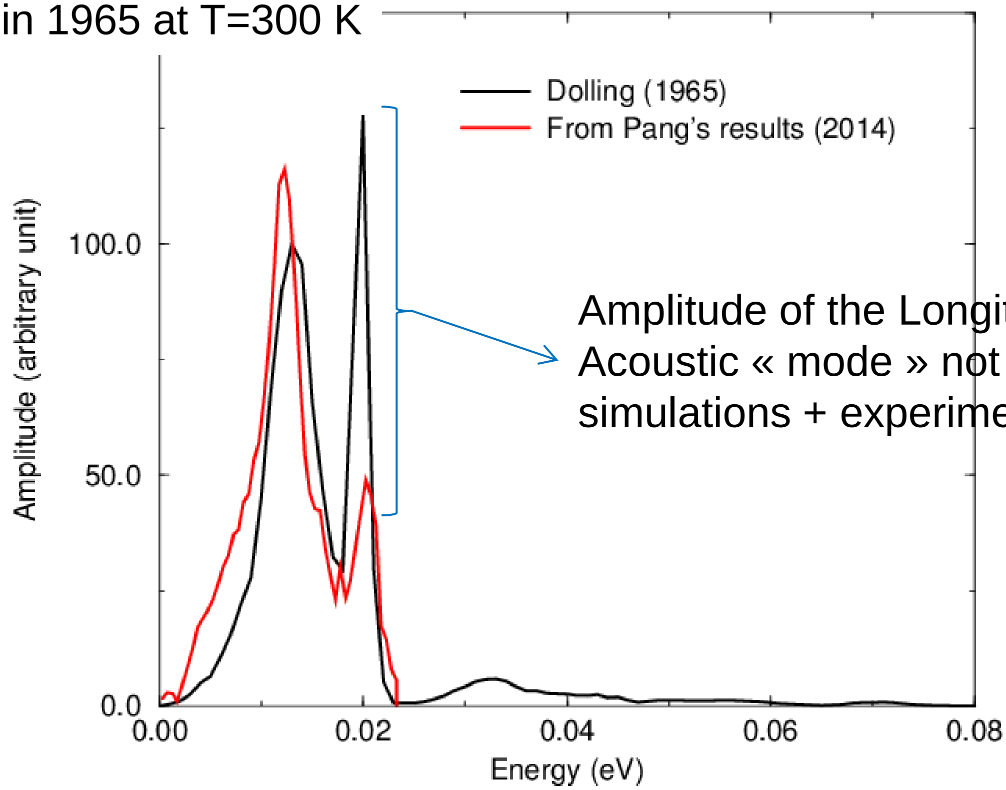


One of the interesting results for neutronic calculations is the <u>shift observed with the temperature</u>

Phonon spectrum

New experimental results from Pang et al. (Phys. Rev. B 89, 115132, 2014)

Comparison with the Dolling's spectrum measured in 1965 at T=300 K



Amplitude of the Longitudinal Acoustic « mode » not confirmed by the simulations + experimental results of Pang

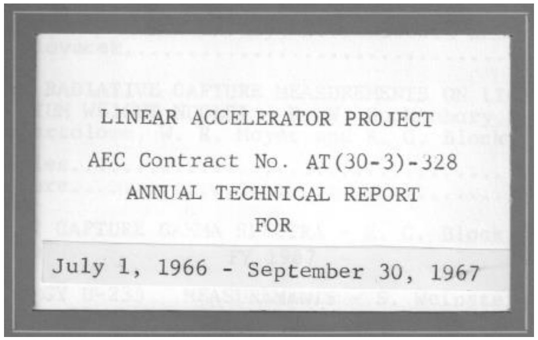
⇒ How to correctly extract the contribution of U in UO2 from Pang's results ?

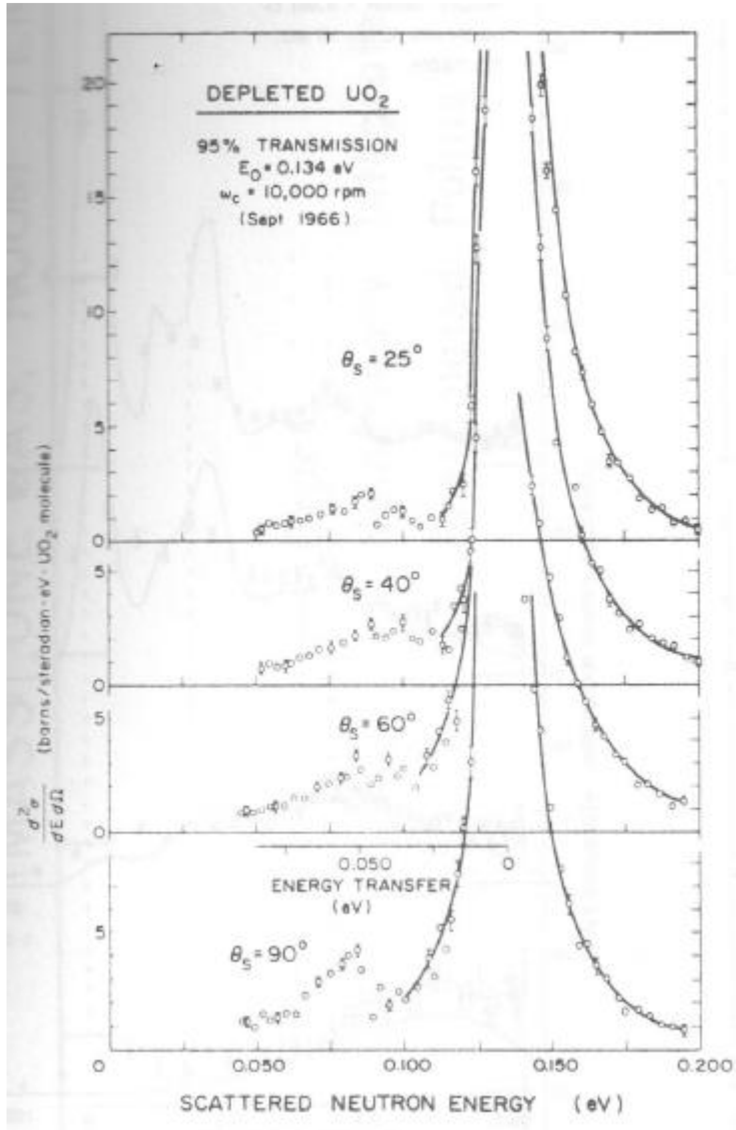
Phonon spectrum

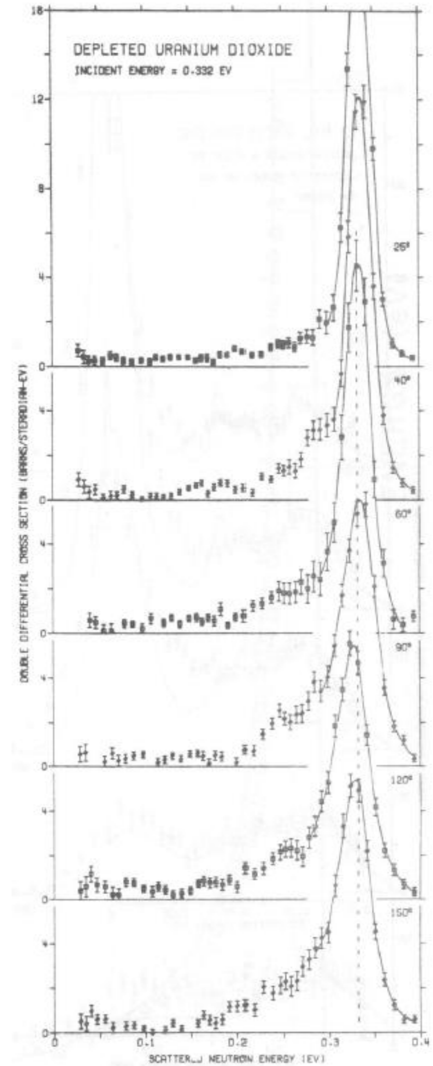
Ongoing activities:

- New « effective temperature law » will be established for neutronic calculations
- U(UO2) libraries (resonance range + TSL) will be produced for APOLLO2 and TRIPOLI-4 codes
- New phonon spectrum from Pang will be tested on old/new UO2 measurements performed at the GELINA facility (transmission measurements)
- LEAPR calculations will be compared to ILL results (end of 2016) + RPI data (1967)

« Old » RPI data …


LINEAR ACCELERATOR PROJECT
AEC Contract No. AT(30-3)-328
ANNUAL TECHNICAL REPORT
FOR
July 1, 1966 - September 30, 1967





NAUSICAA project

Presentations of the NAUSICAA activities during the WPEC/SG-42 meeting (collaboration ILL/IRSN/CEA Cadarache)

- **Vaibhav JAISWAL**, “Measurement of double differential cross section of light water at high temperature and pressure at ILL”

- **Juan Pablo SCOTTA**, “Measurements at Room Temperature and Pressure at ILL”

- **Emmanuel FARHI**, “Total scattering cross section for water: mixing experiments and molecular dynamics”

- **Juan Pablo SCOTTA**, “Propagation of the uncertainties to EOLE benchmarks”

- **Gilles NOGUERE**, “Preliminary covariances obtained for light water with the CONRAD and GROMACS codes”