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NEUTRON RESONANCE SHAPE ANALYSIS OF UO2 DATA MEASURED AT THE GELINA FACILITY BY USING AB-INITIO PHONON SPECTRA

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#### **Resolved Resonance Range (RRR) of the neutron cross sections**

Study of the Doppler effects at low and room temperatures in the first three s-wave resonances of U238 at 6.6 eV, 20.8 eV and 36.6 eV



 $\Rightarrow$  Analysis of transmission data of thin and thick UO2 samples at 23 K and 300 K performed at JRC-Geel

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## **JRC-Geel Time-Of-Flight facilities**



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### **Doppler experimental station**

#### Principle of the measurement of the total cross section



$$T(E) = \int R(E, E') T_{th}(E') dE'$$
$$T_{th}(E) = \exp(-n\sigma_D(E))$$
$$\sigma_D(E) = \int S(E, E') \sigma_{tot}(E') dE'$$

Can be calculated with the Free Gas Model (FGM) or a Cristal Lattice Model (CLM\*)

\*D. G. Nabarejnev, C. Mounier, R. Sanchez "The Influence of Crystalline Binding on Resonant Absorption and Reaction Rates" Nucl. Sci. Eng. 131, 222 (1999)

#### Effect of the Doppler and resolution broadening



The observed width is the quadratic sum of the Doppler, Resolution and natural width of the resonance

 $\Gamma_{\rm exp}^2 \approx \Gamma_D^2 + \Gamma_R^2 + \Gamma_{tot}^2$ 

For U238, the natural width of the resonance is the sum of the elastic, radiation and fission widths

$$\Gamma_{tot} = \Gamma_n + \Gamma_\gamma + \Gamma_f$$

Impact of the Cristal Lattice Model at low and room temperatures calculated with the Dolling spectrum at 6.6 eV



At room temperature, the Doppler contribution is well reproduced with the Free Gas Model and an effective temperature



# Previous Neutron Resonance Shape Analysis were mainly performed with the Dolling spectrum measured at 300 K

 $\Rightarrow$  not suitable for low temperature

### New calculated spectra at room temperature are available

- $\Rightarrow$  Judy Pang (Oak Ridge)
- $\Rightarrow$  North Caroline South University (NCSU) —

Agreement with the SNS data is improved



#### In this work, we use recent spectra calculated at 23 K and 300 K by Pablo Maldonado

Calculation details can be found in the following article on NpO2

PHYSICAL REVIEW B 93, 144301 (2016)

#### Crystal dynamics and thermal properties of neptunium dioxide

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Density of states of U in UO2

#### In this work, we use recent spectra calculated at 23 K and 300 K by Pablo Maldonado



**Density of states of U in UO2** 

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#### First step : Analysis of the transmission data (thick sample) at 300 K with the CLM

Ajustement of the resonance energies and neutron widths with the SAMMY code (ORNL)



Comparison with the latest neutron widths established at JRC-Geel (available in JEFF-3.3)

#### First step : Analysis of the transmission data (thick sample) at 300 K with the CLM



	6.6 eV	20.8 eV	36.7 eV
$\Gamma_{n}(JEFF ext{-}3.3)$	1.49 meV	10.08 meV	33.59 meV
$\Gamma_{\sf n}$ (This work)	1.51 meV	10.07 meV	32.92 meV
$\Gamma_{n}$ (This work)/ $\Gamma_{n}$ (JEFF-3.3)-1	+1.3%	-	-2.0%

 $\Rightarrow$  Excellent agreement that remains within the limit of the experimental uncertainties

#### Second step : Analysis of the transmission data (thick sample) at 23 K with the CLM



Good agreement with the data measured at low temperature, but ...

#### Second step : Analysis of the transmission data (thick sample) at 23 K with the CLM



#### Second step : Analysis of the transmission data (thick sample) at 23 K with the CLM



Further works are needed to explain the differences ...



# It is the first time that the JRC-Geel data at 23 K were analysed with an appropriate phonon spectrum $\Rightarrow$ How to explain the observed differences ?

- New measurements at low temperature are needed
- Repeat such calculations for NpO2 data measured JRC-Geel at 77 K
- Clarify the limits of the Crystal Lattice Model implemented in SAMMY
- Add "quantum correction" from Abe
- Comparison with the REFIT and CONRAD codes
- Radiation widths should be increased
- ...