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Effect of thermal resonant treatment on keV scattering cross sections

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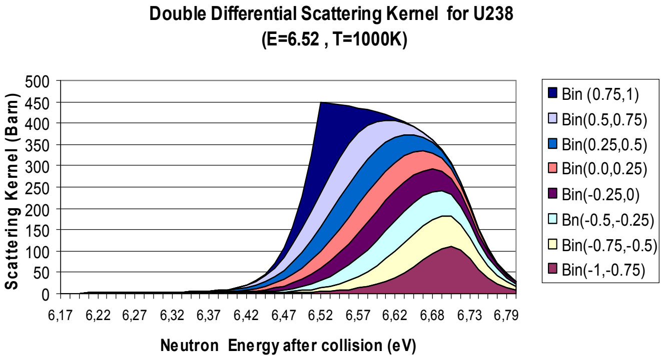
OM based thermal scattering?

- The new ENDF -VIII library replaces the asymptotic model and the energy ranges based on the OM.
- In the case of Fe 56-
- ENDF_VIII (ENDF_ VII) , JEFF3.1.2

3958	2	2631	4	2				1782	2	2631	4	2
0.000000+0	1.000000-5	0	0	6	2631			0.000000+0	1.000000-5	0	0	4
5.877681-5	1.316087-5	1.28475-12	1.03868-11	9.20038-21	0.000000	02631		0.000000+0	0.000000+0	0.000000+0	0.000000+0	2631
0.000000+0	5.000000+3	0	0	8	2631			0.000000+0	1.584600+3	0	0	4
5.892811-4	2.119867-4	1.00149-10	1.231904-8	2.58131-16	1.09360-16	2631		0.000000+0	0.000000+0	0.000000+0	0.000000+0	2631
6.65078-24	0.000000+0	2631	4	2				0.000000+0	1.170900+4	0	0	4
0.000000+0	1.000000+4	0	0	8	2631			1.114400-2	2.867900-5	-6.457300-8	1.40440-11	2631
1.542063-3	5.167644-4	1.105931-9	2.598255-7	5.77867-15	3.75311-18	2631		0.000000+0	1.503400+4	0	0	4
7.62588-22	0.000000+0	2631	4	2				-0,0045804	-1.4703-4	1.742400-7	2.90070-10	
0.000000+0	1.100000+4	0	0	8	2631							
1.756560-3	5.784115-4	1.655324-9	3.903650-7	1.17337-14	9.69385-16	2631						

- Even if the Legendre moments are quite “asymptotic” the theory is questionable

The full free gas based model vs. the full solid state



<u>IDEAL GAS KERNEL: ENERGY DEPENDENT $\sigma_s(E_r)$</u>

$$\sigma_s^{T}(E \to E', \vec{\Omega} \to \vec{\Omega}') =$$

$$\frac{1}{4\pi E}\sqrt{\frac{A+1}{A\pi}} \int_{\epsilon_{max}}^{\infty} d\xi \int_{\tau_0(\xi)}^{\tau_1(\xi)} d\tau$$

$$\left[\frac{(\xi+\tau)}{2}\right]\left(\frac{A+1}{A}\right)^2 \sigma_s \left[\left(\frac{A+1}{A^2}\right)\frac{[\xi+\tau]^2}{4} k_B T\right]$$

$$\exp\left\{v^2 - \left[\frac{(\xi+\tau)^2}{4A} + \frac{(\xi-\tau)^2}{4}\right]\right\}\left[\frac{\epsilon_{max}\epsilon_{min}(\xi-\tau)^2}{B_0 sin\hat{\varphi}}\right]$$

Solid state based expression of Word & Trammel (1980)

$$\frac{\mathrm{d}^2\sigma_R}{\mathrm{d}\Omega \mathrm{d}E} = \frac{v}{2\pi}\left(\frac{\Gamma_n}{2k_i}\right)^2 \left(\frac{E_f}{E_i}\right)^{1/2} \int_{-\infty}^{\infty} \mathrm{d}T \exp(+iET) \int_0^{\infty} \mathrm{d}t \exp[a(t)] \int_0^{\infty} \mathrm{d}t'$$
$$\times \exp[a^*(t')] \times W(T, t, t'),$$

$$W(T, t, t') = \Big\langle \exp\left[-i\vec{k}_i \vec{r}(T-t')\right] \exp\left[i\vec{k}_f \vec{r}(T)\right]$$
$$\exp\left[-i\vec{k}_f \vec{r}\right] \exp\left[i\vec{k}_i \vec{r}(-t)\right]\Big\rangle.$$

$$a(t) = -i(E_r - E_i - i\Gamma/2)\mathrm{t}.$$

From John Rowlands Lectures:

Published Studies on Resonance Scattering in Solids

1. Shamaoun and Summerfield (1990)

- By calculating the "short collision time approximation" to the equations, they show that when this approximation is valid for both the Doppler broadening of the resonance shape and for the calculation of the secondary distribution, the Lamb approximation applies to both.
- (The model they use is a for harmonic crystal with cubic symmetry.)
- They point out that in the “short collision time approximation” the scattering equation they derive is of the same form as that given for an ideal gas by Holger St John (Thesis 1979).
- *A question to be considered is whether the condition for the validity of the short collision time approximation for the secondary energy distribution is the same as Lamb's condition for this to apply to the formation of the compound nucleus.*

From John Rowlands Lectures:

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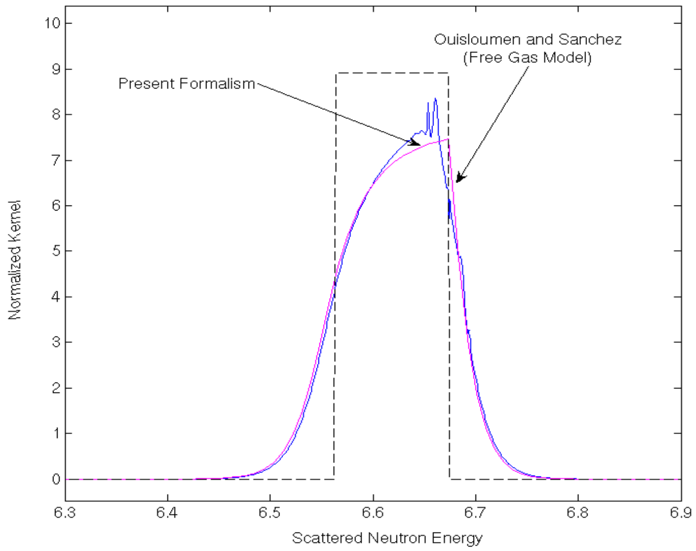
Published Studies on Resonance Scattering in Solids
2. Naberejnev (2000)

- Naberejnev calculates the energy distribution of scattered neutrons at points above and below the peak of the U238 resonance at 6.7 eV using his approximate model, MUPA. He finds the distributions are more similar to those calculated for scattering by a constant cross-section than to those calculated using the free gas model.
- At 300 K the free gas model (Ouisloumen) gives an upscattering probability at E_i = 6.52 eV of 45.69% and at E_i = 7.2 eV, of 16.5%.
- Naberejnev's MUPA formalism predicts upscattering probabilities
- equal to 22.6% and 16.5%. (At 7.2 eV resonance effects are small)
- Hence, according to Naberejnev, the free gas model overestimates upscatter probabilities below the resonance peak./
(See R. Dagan ANE 2005 and Shamaoun and Summerfield 1990)

Energy dependent Solid state effect

- Word and Trammel equation was never solved directly due to mathematical complexity. A. Courcelle and John Rowlands suggested a new formalism (Courcelle, Rowlands 2007)
- It combined the free gas resonance solver approach with a crystal lattice model for the inclusion of the solid state effect.

- The solution of Courcelle and Rowlands was the most advanced milestone before a direct solution for the very oscillating Word and Trammel   expression.



Solid state and Resonant treatment

Phonon Expansion: $S(\alpha,\beta) = e^{-\alpha\lambda} \sum_{n=0}^{\infty} \frac{1}{n!} [\alpha\lambda]^n \mathcal{T}_n(\beta)$

$\mathcal{T}_0(\beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\beta t}\, dt = \delta(\beta);$

$\mathcal{T}_1(\beta) = \frac{P(\beta) e^{-\frac{\beta}{2}}}{\lambda};$

$\mathcal{T}_n(\beta) = \int_{-\infty}^{\infty} \mathcal{T}_1(\beta')\mathcal{T}_{n-1}(\beta - \beta')\, d\beta';$

$\mathcal{T}_n(\beta) = e^{-\beta} \mathcal{T}_n(-\beta);$

$\beta = \frac{E - E'}{kT};\ \alpha = \frac{E' + E - 2(EE'\mu)^{\frac{1}{2}}}{AkT};$

$P(\beta) = \frac{\rho(\beta)}{2\beta \sinh\left(\frac{\beta}{2}\right)};\ \lambda = \int_{-\infty}^{\infty} P(\beta) e^{-\frac{\beta}{2}}\, d\beta;$

$\rho(k,k',+t) = \frac{k \cdot k'}{2M} \int_0^{\infty} \frac{\rho(\omega)}{\omega} \left[\coth\left(\frac{\omega}{2kT}\right)\cos(\omega t) - i\sin(\omega t)\right] d\omega$

Resonant treatment

$$\sigma_s^T(E \to E', \Omega \to \Omega') =$$

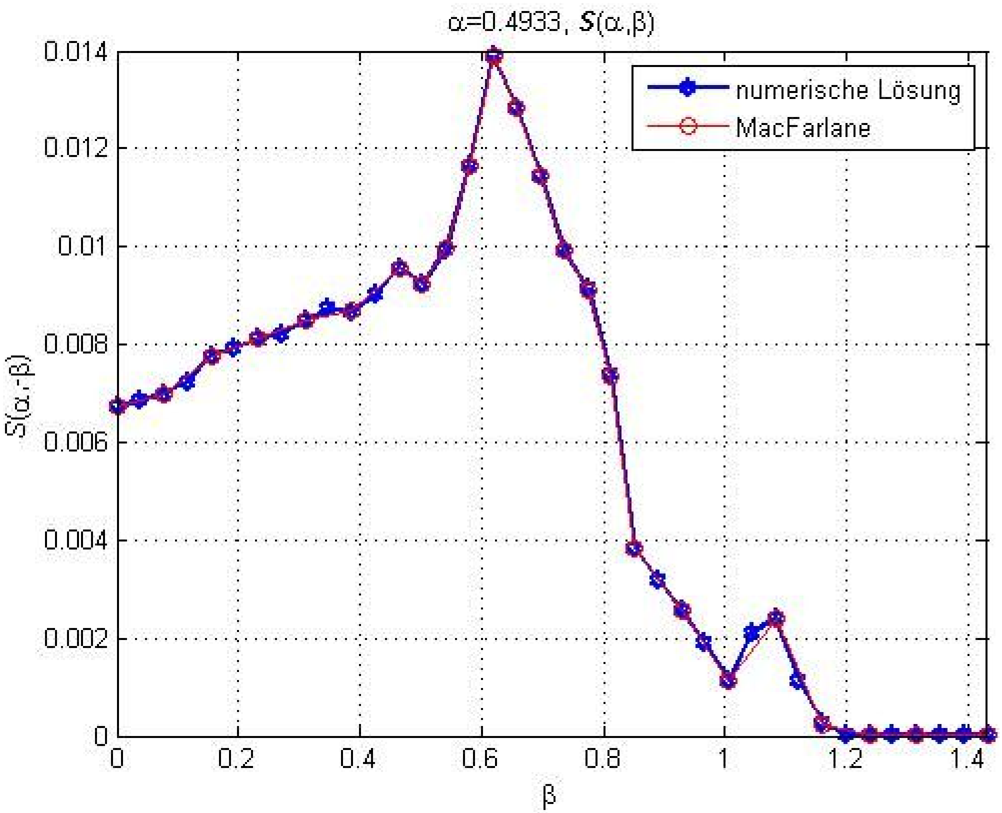
$$\frac{1}{4\pi E} \sqrt{\frac{A+1}{A\pi} \int_{max}^{\infty} d\xi \int_{\eta 0}^{\eta} d\tau \left(\frac{(\varepsilon+\tau)}{2}\left(\frac{A+1}{A}\right)^2\right.}$$

$$\left.\sigma_s\left[\frac{A+1}{A^2}\frac{[\varepsilon+\tau]^2}{4} k_b T\right] \exp\left(\vartheta^2 - \left[\frac{(\xi+\tau)^2}{4A} + \frac{[\xi-\tau]^2}{4}\right]\right]\right.$$

$$\frac{emaxemin(\xi-\tau)^2}{B_0 \sin\varphi}$$

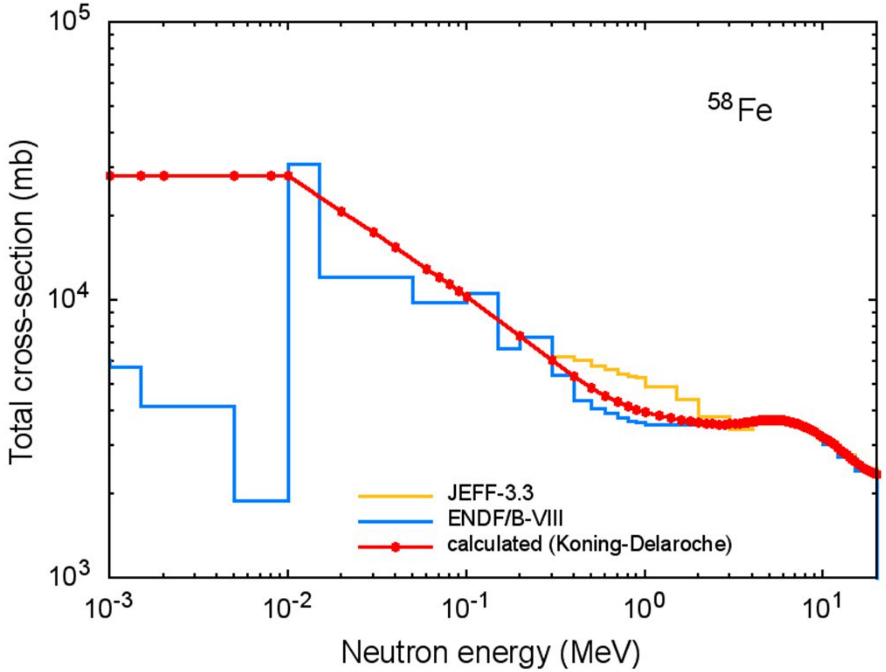
example: Comparison Matlab against numerical solution

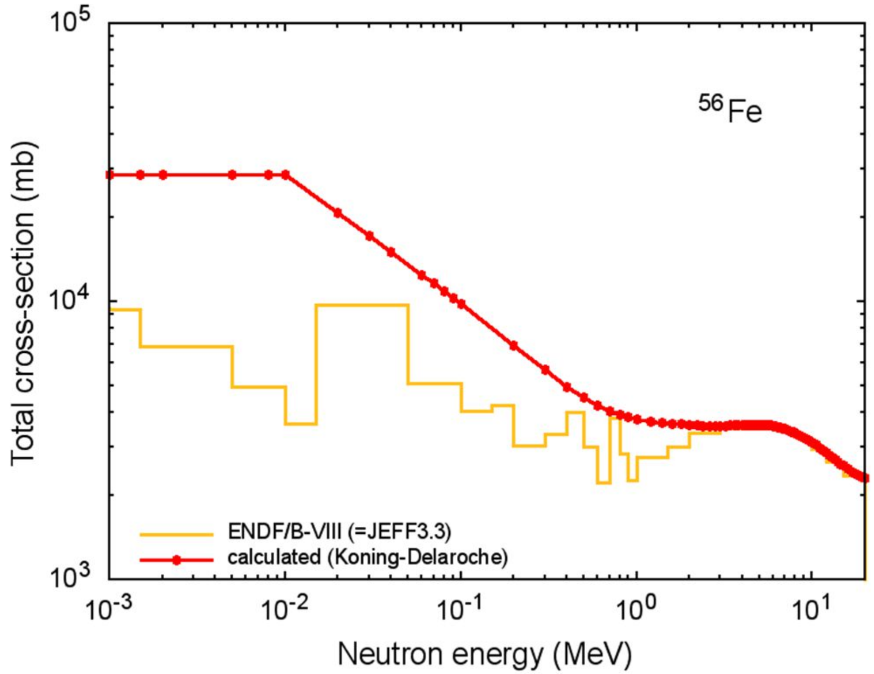
$$S(\alpha,\beta) = \exp(-\alpha\lambda)\sum_{n=0}^{\infty}\frac{1}{n!}[\alpha\lambda]^n{}_nT(\beta)$$



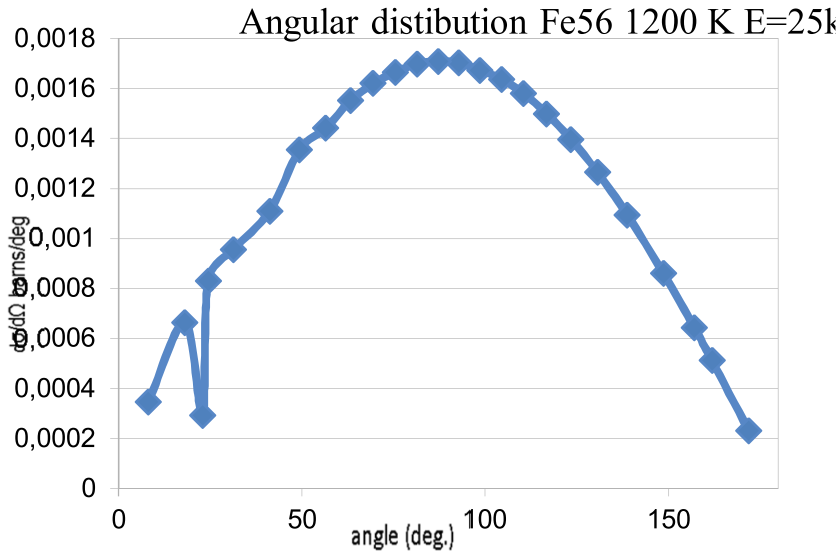
comparison between the OM (Koning-Delaroche) vs JEFF3.3 or/and ENDF/B-VIII library for Fe56 and Fe58.

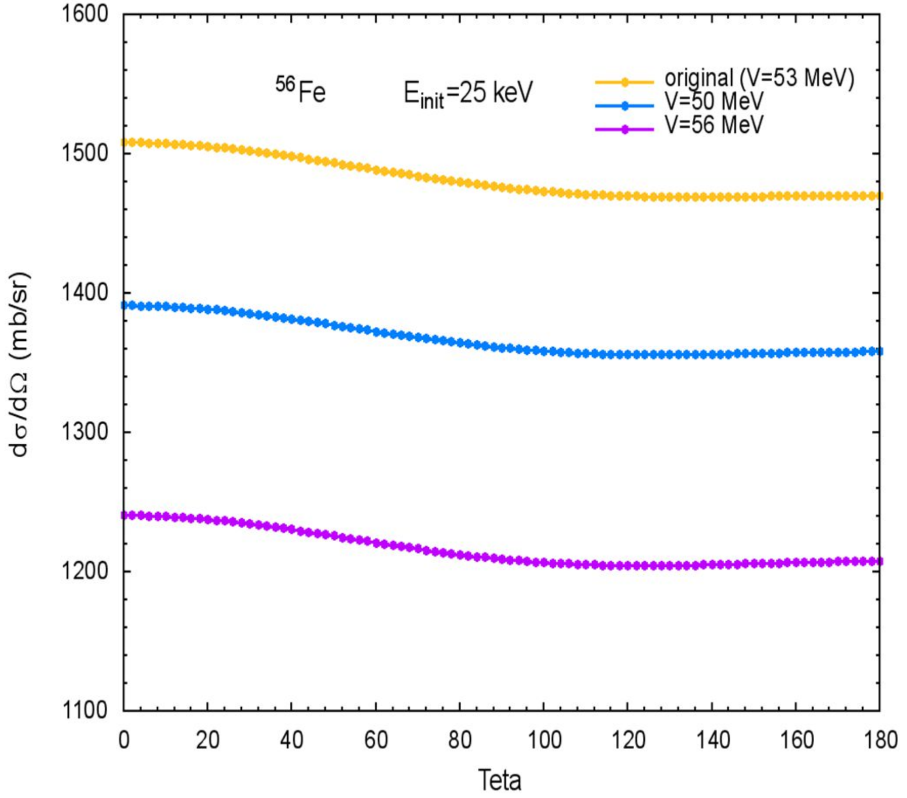
Differences up to factor 6 and 10 in Fe56 and Fe58 respectively in the total cross sections at energy range of tenth of KeV



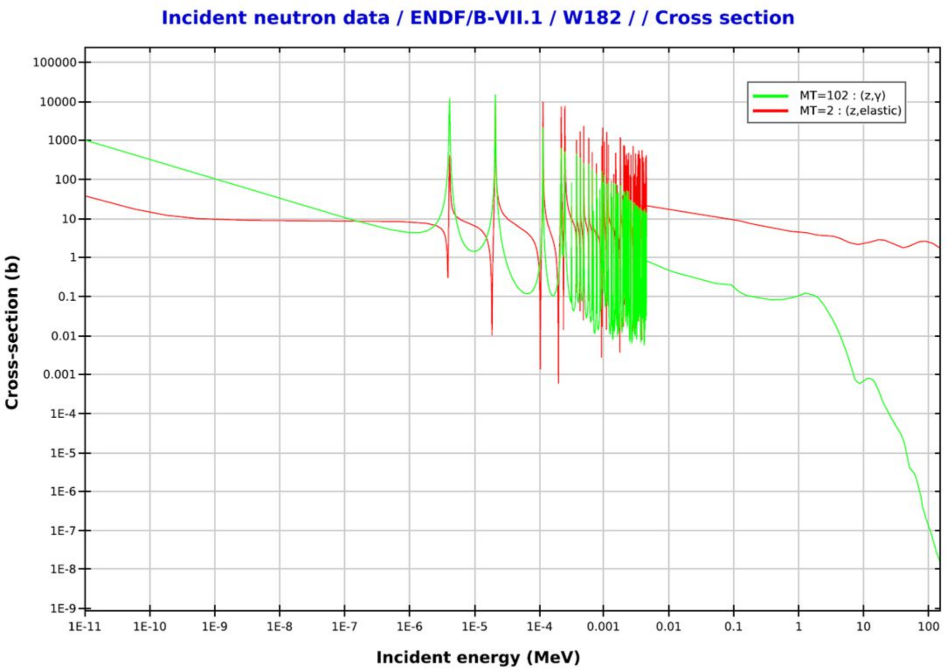


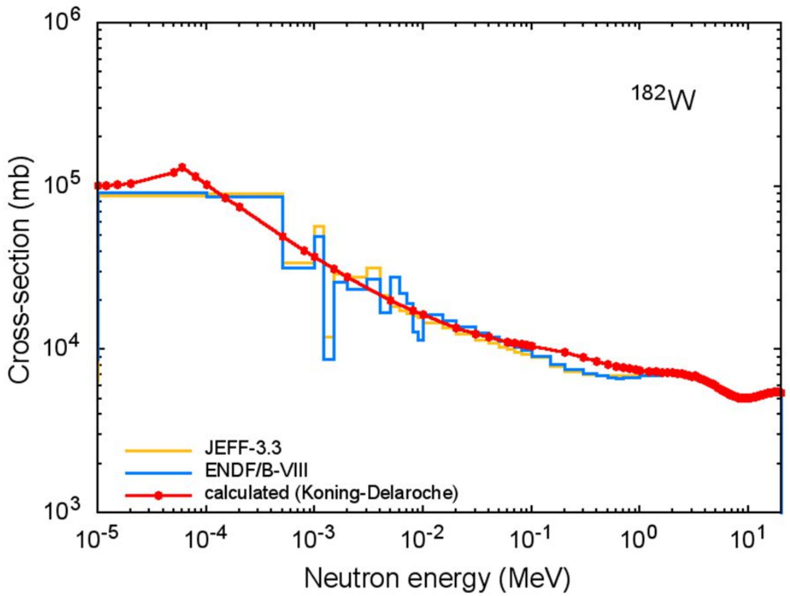
Exact Temperature and energy dependent Angular distribution vs. OM for Fe56



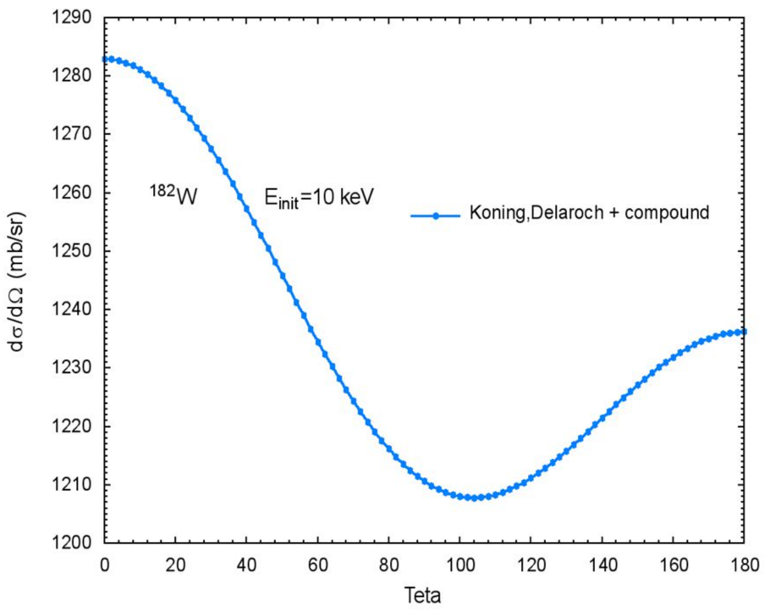


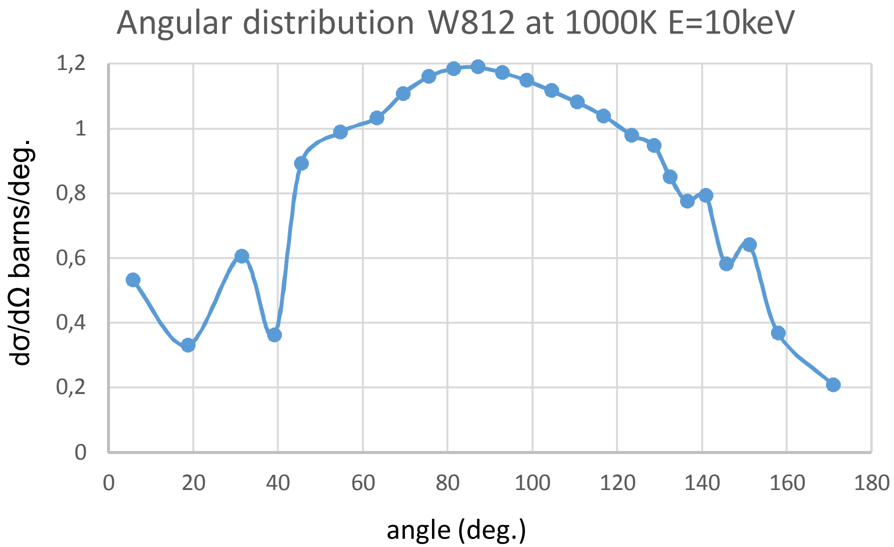
W182: Comparison between nuclear data Libraries and OM based cross sections





Exact Temperature and energy dependent Angular distribution vs. OM for W182





Experimental evidence for energy dependent Angular distribution

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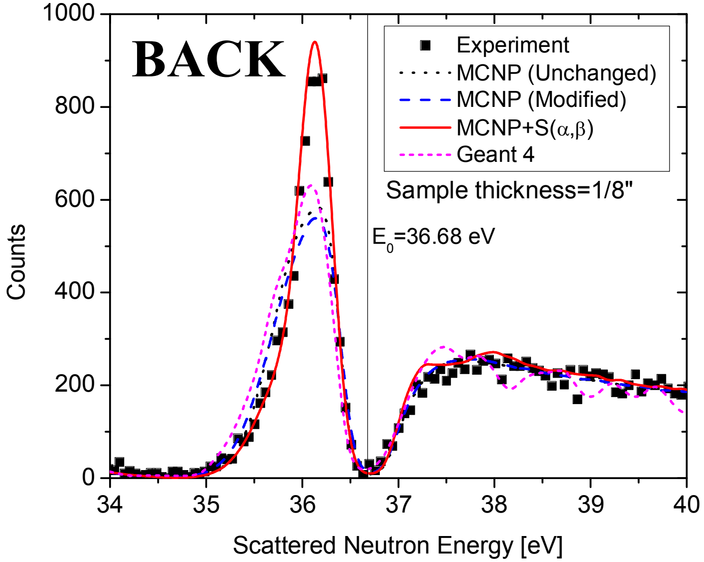
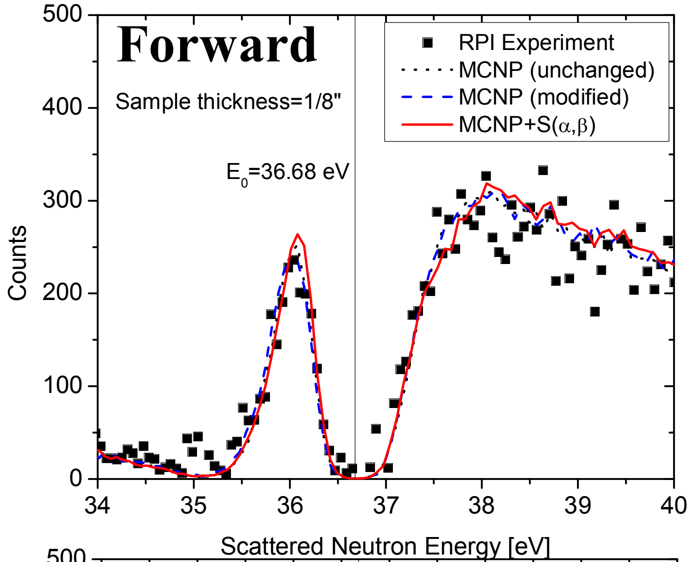
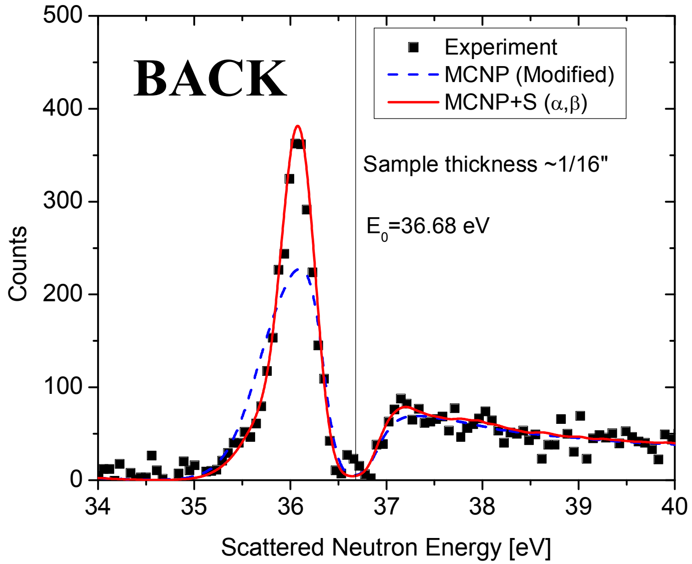
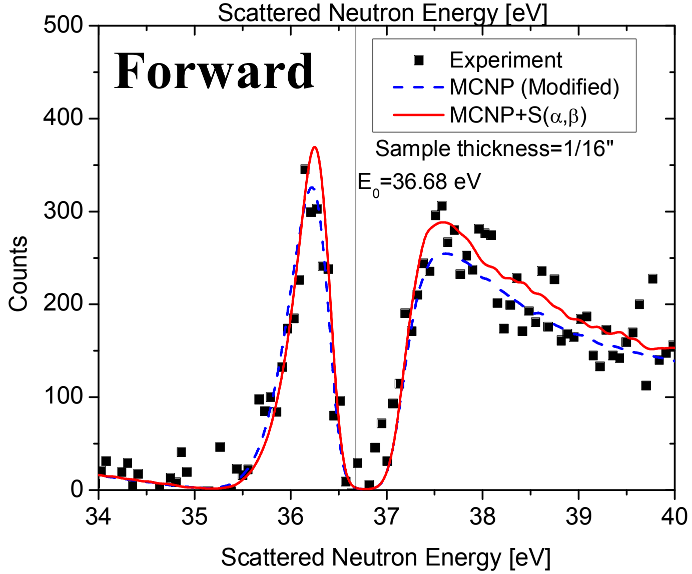


Thick Sample





Thin Sample



Summary

- Thermal scattering should involve the energy dependency. Suggestions by J. Rowlands could be a reference case.

- Higher energy should also in principle involves the energy dependency in its accurate mode and probably the thermal scattering treatment should be extended and "replaced" by a adequate theory which the OM can't comply with, due to its temperature independent and average definition.
- More experiments in the tenth of KeV range are inevitable to understand the range of different theories and their importance.