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Summary, conclusions and recommendations of the CM on EXFOR Compilation of Thermal Neutron Scattering Data

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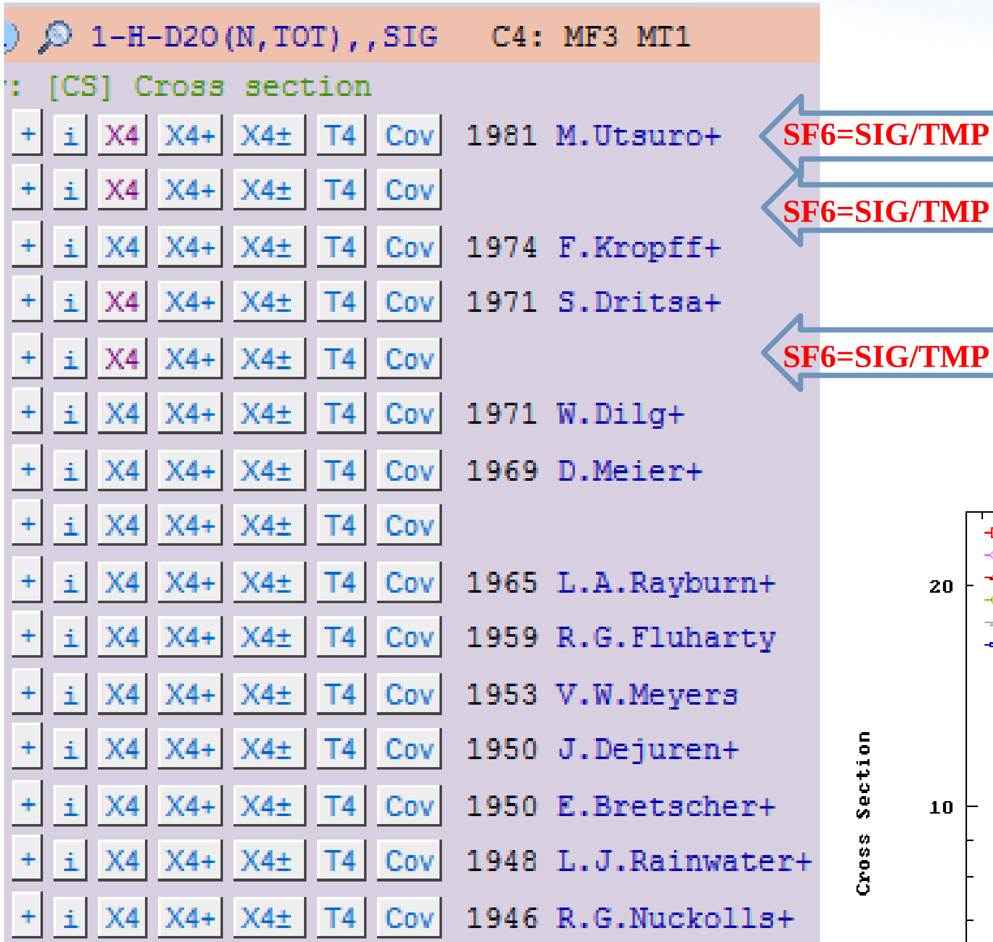
Outline

- Motivation
- Neutron interactions at thermal energies
- CM overview
- CM conclusions and recommendations

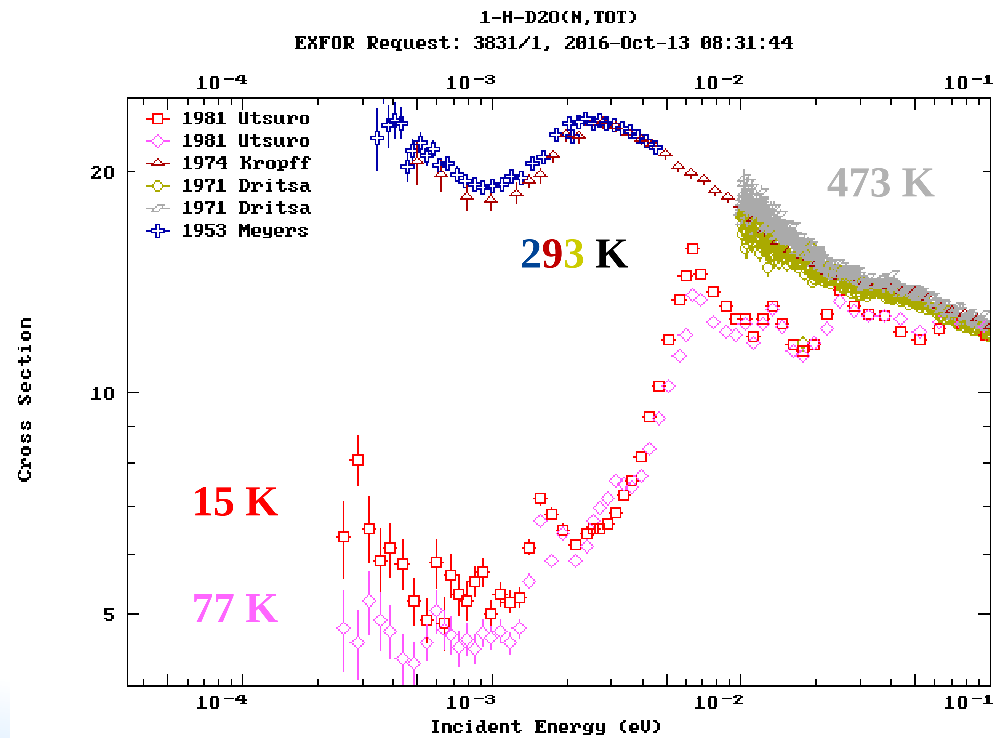
Compilation of cross sections at thermal energies - I



1-H-D2O(N,TOT),,SIG C4: MF3 MT1

[CS] Cross section

+	i	X4	X4+	X4±	T4	Cov	1981 M.Utsuro+	SF6=SIG/TMP
+	i	X4	X4+	X4±	T4	Cov		SF6=SIG/TMP
+	i	X4	X4+	X4±	T4	Cov	1974 F.Kropff+	
+	i	X4	X4+	X4±	T4	Cov	1971 S.Dritsa+	
+	i	X4	X4+	X4±	T4	Cov		SF6=SIG/TMP
+	i	X4	X4+	X4±	T4	Cov	1971 W.Dilg+	
+	i	X4	X4+	X4±	T4	Cov	1969 D.Meier+	
+	i	X4	X4+	X4±	T4	Cov		
+	i	X4	X4+	X4±	T4	Cov	1965 L.A.Rayburn+	
+	i	X4	X4+	X4±	T4	Cov	1959 R.G.Fluharty	
+	i	X4	X4+	X4±	T4	Cov	1953 V.W.Meyers	
+	i	X4	X4+	X4±	T4	Cov	1950 J.Dejuren+	
+	i	X4	X4+	X4±	T4	Cov	1950 E.Bretscher+	
+	i	X4	X4+	X4±	T4	Cov	1948 L.J.Rainwater+	
+	i	X4	X4+	X4±	T4	Cov	1946 R.G.Nuckolls+	



Compilation of cross sections at thermal energies - II

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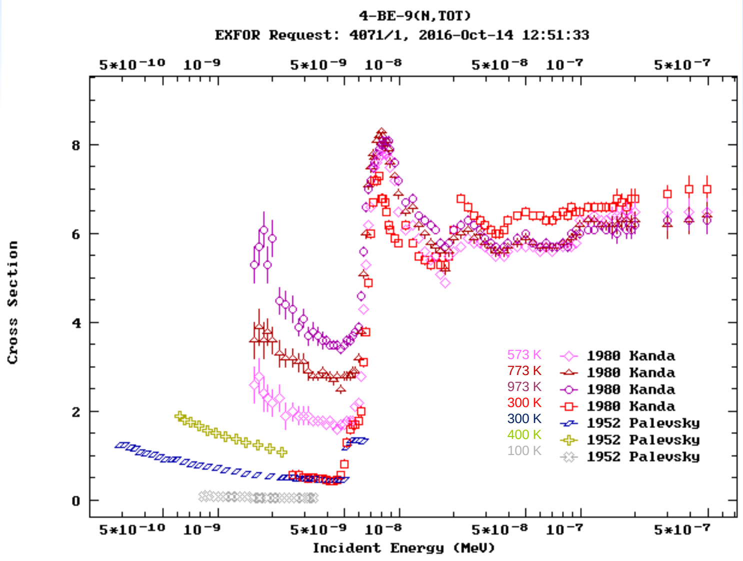
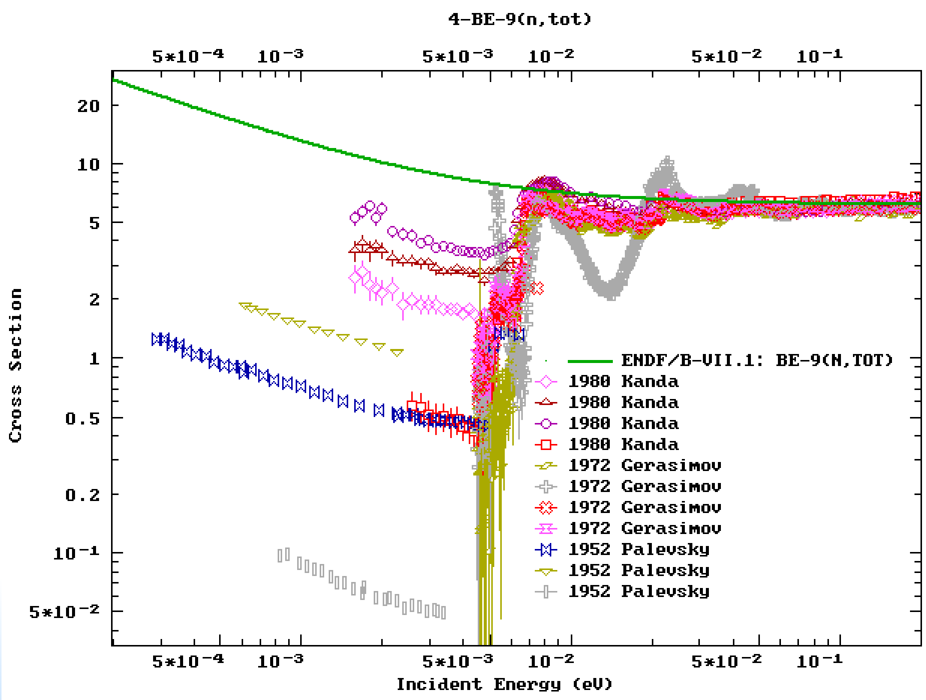
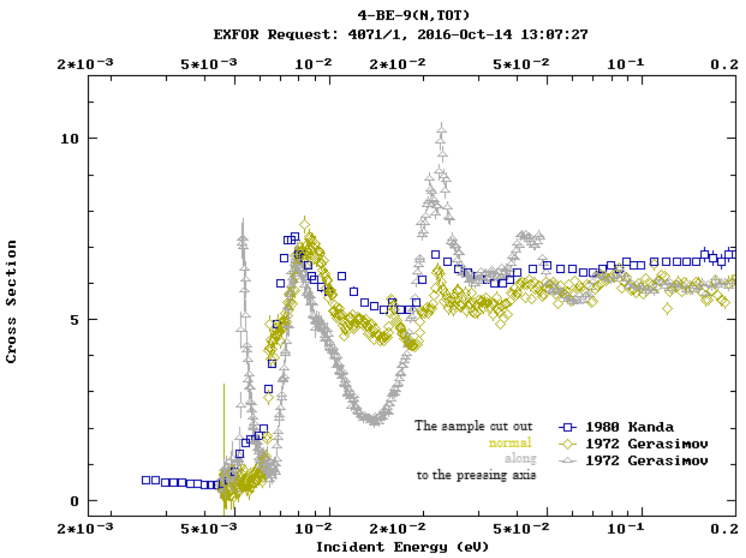
Below 0.1 eV the CS depends on:

- bounding of atoms
- temperature
- sample properties and orientation







Thermal-neutron scattering data (applications) -I

- Nuclear technologies
  - nuclear reactor design (TSL data are needed for both the moderator and to evaluate crystal lattice effects in UOX fuel.
  - analysis of the nuclear criticality safety
  - accelerator driven sub-critical systems for waste incineration

Effects of thermal data on resonance analysis

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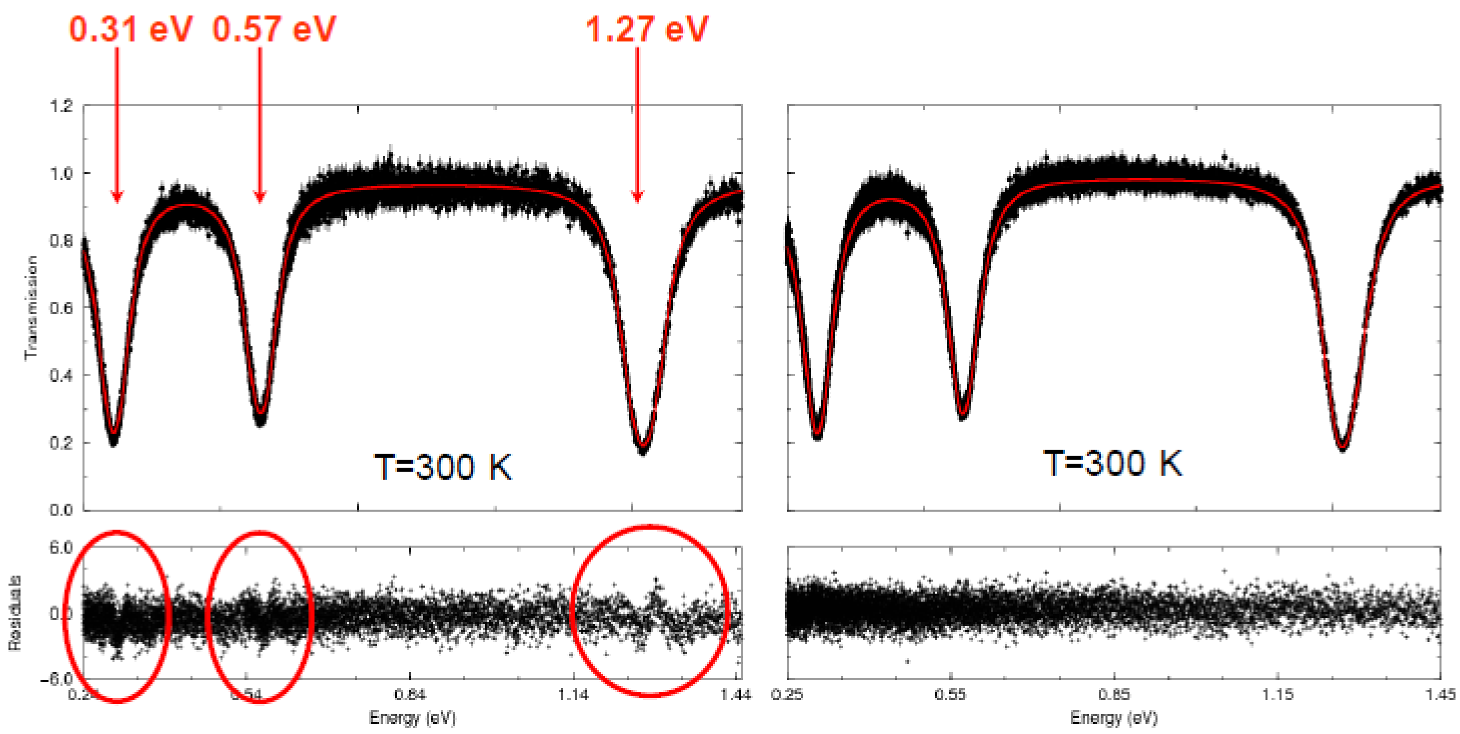
Am241 transmission measurements at the GELINA facility, IRMM, Geel

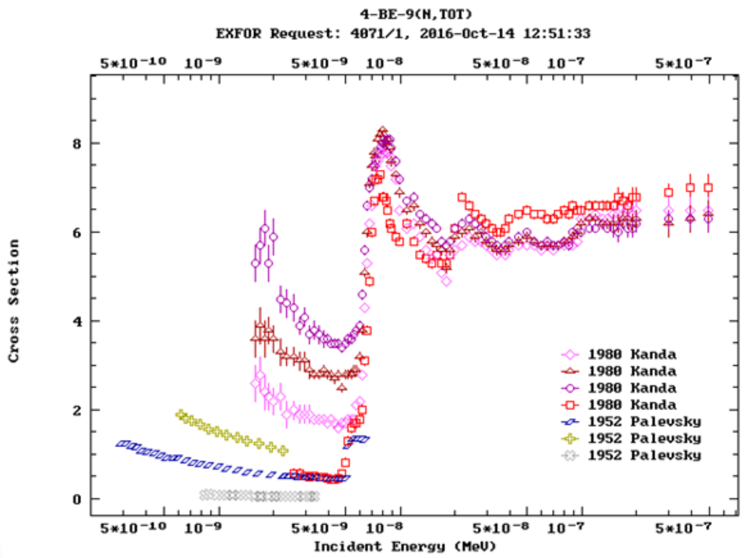
C. Lampoudis et al. Eur. Phys. J. Plus, 128, 86 (2013)



Free Gas Model (FGM)
with an effective temperature

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

- Many questions emerge from the **WPEC SG-40** (CIELO) related to the impact of the thermal scattering data on criticality benchmarks
- Neutron beam spectral shaping (filtering)



Thermal-neutron scattering data (applications) -II

- Neutron source characterisation
- Medical applications
- Material science research using thermal and cold neutrons.

The wavelength of neutrons with energy of 80 meV is 1 Å.

- the $\lambda \approx$ distance between atoms.
- the E $\approx$ fundamental excitations in condensed matter such as phonons, magnons, and other basic excitations.

=> neutrons are simultaneously sensitive to both atomic structure and dynamics and thus probe the space–time correlation function of the system under study.

Material structure measurements

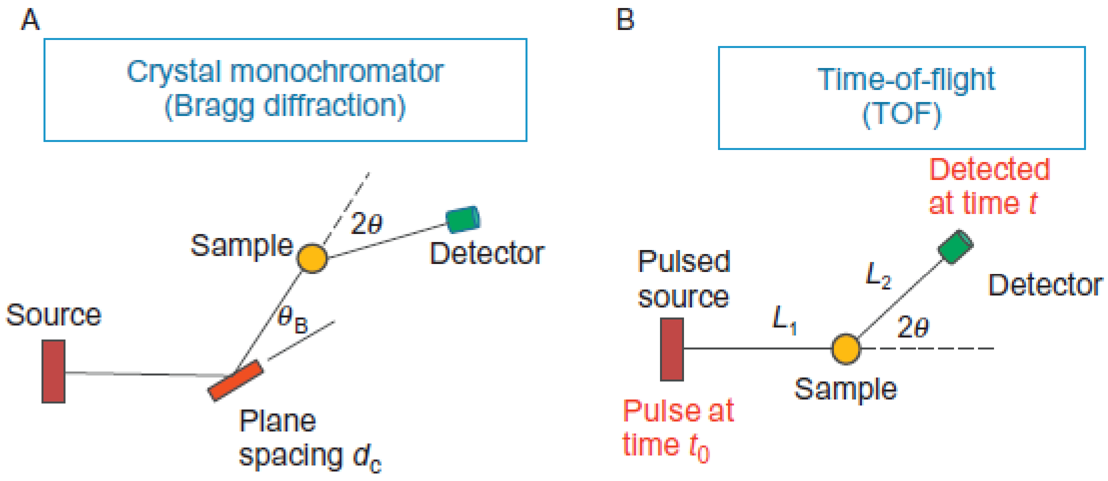


FIGURE 3.1 Diffraction technique: (a) crystal-monochromator diffraction and (b) time-of-flight diffraction.

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Measurement techniques to study both, the structure and the dynamics

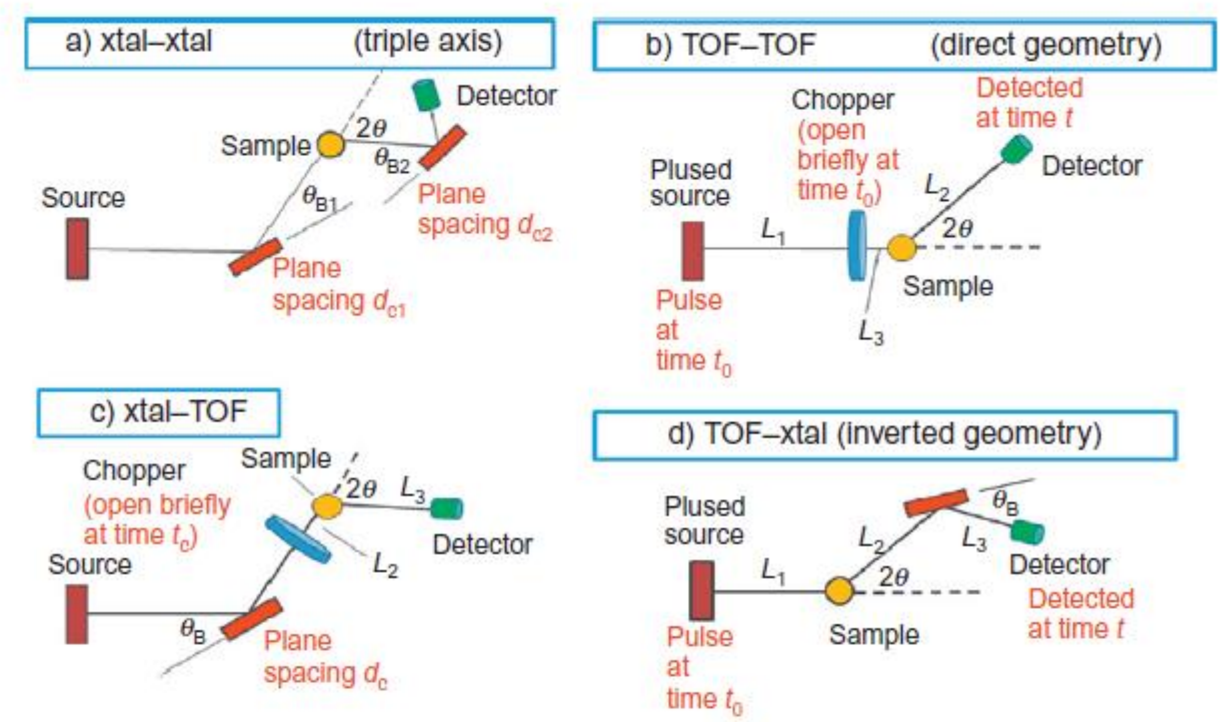

FIGURE 3.2 Typical inelastic scattering techniques.

Recommendations of the 30th INDC meeting

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- Support non-OECD contributions to new evaluated and experimental data for TSL
- Thermal data (phonon spectrum, S(αβ) are needed for various nuclear reactors moderators and structural materials. These data are crucial for a proper knowledge of a light water reactor's spectrum.
- To validate evaluations in the resolved range, time of flight experiments are needed in the temperature interval from a few K to 1000 K. Low temperature measurements could disentangled the effect of crystal lattice on the knowledge of resonance parameters for major isotopes (e.g. 238U and 239,240,241Pu)

Recommendations of the 30th INDC meeting - II

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- Thermal scattering data are required for Be, BeO and BeF4 related to neutronics calculations
- Thermal scattering data are required for material science research using cold neutrons.
- The lack of studies and data of thermal neutron scattering in organic tissues, which might have a large impact on neutron dosimetry in BNCT where the "therapeutic" neutrons are thermal. Similar impact could be found in the practice of neutron Brachytherapy and Radiation Protection.

WPEC-SG42 recommendations

Link with the experimental database EXFOR

⇒ How to test and improve TSL data ?

- **Integral experiments** are sensitive to various nuclear data
- Direct comparison with **experimental total cross section** is easy but not enought
- Direct comparisons with **double-differential data** are difficult ⇒ the simulation of the experimental set-up with Monte-Carlo codes are often impossible (missing experimental information)

This issue has to be discussed at AIEA in order to propose long term solutions for storing and communicating precise experimental information, MCNP inputs … (solutions already exist for criticality, propagation and reactor benchmarks with ICSBEP, SINBAD and IRPHE)

IAEA/TSL library

INDL/TSL
IAEA Nuclear Data Library / Thermal Scattering Law

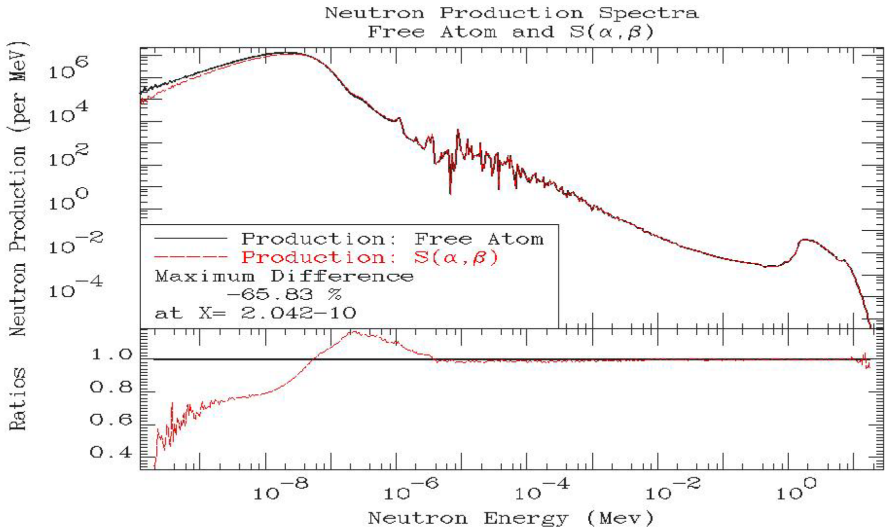
Available documentation for the IAEA/TSL library

- Library description for H(H2O), D(D2O), H(Zr H) and graphite. .
- Cullens pin-cell benchmark analysis document.
- Library validation study presented at the conference in Portoroz in September 2004.

MAT	Compound	Description	ENDF File	ENDF zip File	ACE File	ACE zip File
1	H(H2O)	hydrogen bound in water	indl_H_H2O.dat	indl_H_H2O.zip	H_H2O.ace	H_H2O-ace.zip
2	para-H	para-hydrogen	indl_para-H.dat	indl_para-H.zip		
3	ortho-H	ortho-hydrogen	indl_ortho-H.dat	indl_ortho-H.zip		
7	H(ZrHx)	hydrogen bound in zirconium hydride	indl_H_ZrH.dat	indl_H_ZrH.zip		
8	H(TiH2)	hydrogen bound in titanium hydride	indl_H_TiH2.dat	indl_H_TiH2.zip		
9	H(YH2)	hydrogen bound in yttrium hydride	indl_H_YH2.dat	indl_H_YH2.zip		
10	H(CeH2)	hydrogen bound in cerium hydride	indl_H_CeH2.dat	indl_H_CeH2.zip		
11	D(D2O)	deuterium bound in heavy water	indl_D_D2O.dat	indl_D_D2O.zip		
12	para-D	para-deuterium	indl_para-D.dat	indl_para-D.zip		
13	ortho-D	ortho-deuterium	indl_ortho-D.dat	indl_ortho-D.zip		
31	C	graphite	indl_graphite.dat	indl_graphite.zip		

“How Accurately Can We Calculate Thermal Systems”

INDC(USA)-107(UCRL-TR-203892)



Objectives:

How accurately variety of neutron transport code packages (**code and cross section libraries**) can calculate simple reactor lattice integral parameters, such as K-eff, for systems that are sensitive to thermal neutron scattering?

Conclusion:

The effects of the thermal scattering models is important!

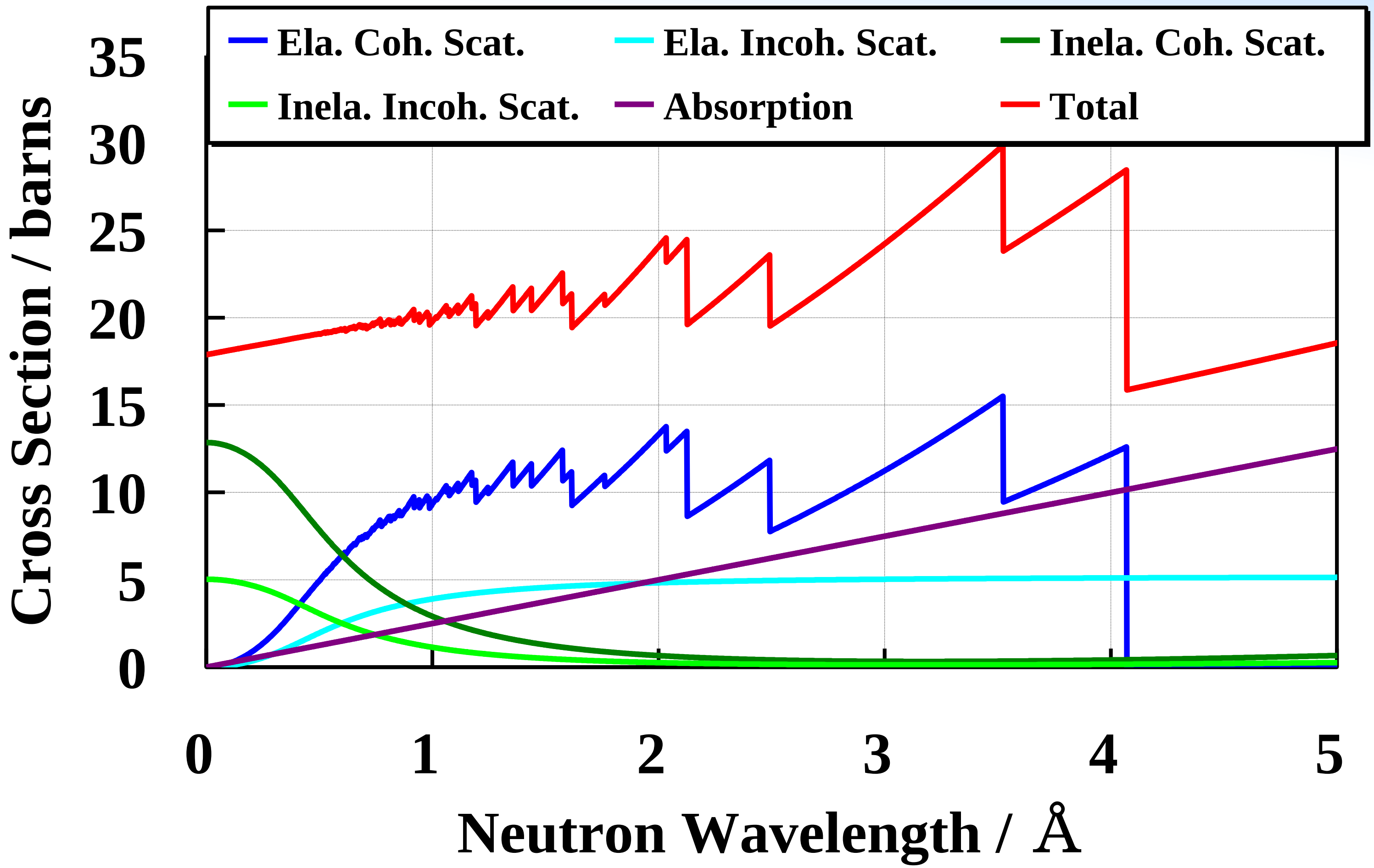
Compilation of TSL quantities

Thermal-Neutron Scattering data are included in the scope of EXFOR compilation. However, the completeness and the consistency of the compiled data need to be verified.

Do we need to revise the existing compilation rules?

BA,SIG/TMP	B	(Bound-atom cross section,	3000023600173
BA,AMP	L	(Bound-atom scattering amplitude)	3000023600963
BA/COH,AMP	L	(Bound-atom coherent scattering amplitude)	3000023600964
BA/PAR,AMP	L	(Partial bound-atom scattering amplitude)	3000023600965
FA,SIG	B	(Free-atom cross section)	3000023600253
FA,SIG/TMP	B	(Free-atom cross section,	3000023600254
FA/COH,SIG	B	(Free-atom coherent scattering cross	3000023600257
FA/INC,SIG	B	(Free-atom incoherent scattering cross	3000023600259
FA,AMP	L	(Free-atom scattering amplitude)	3000023600969
FA/INC,SIG	B	(Free-atom incoherent scattering cross	3000023600259
INC,SIG	B	(Incoherent scattering cross section)	3000023600263
INC,AMP	B	(Incoherent scattering amplitude)	3000023600971
COH,SIG	B	(Coherent cross section)	3000023600185
FA/COH,SIG	B	(Free-atom coherent scattering cross	3000023600257
BA/COH,AMP	L	(Bound-atom coherent scattering amplitude)	3000023600964
COH,AMP	L	(Coherent scattering amplitude)	3000023600966
COH/IM,AMP	L	(Coherent scattering amplitude (imaginary	3000023600967

Calculated cross section $\sigma_{tot}(\lambda)$ of Ni under the condition of isotropic, no-strain, and no-extinction



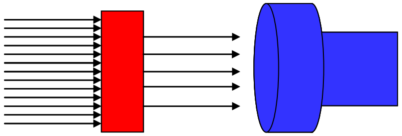
Cf: CRIPO (by Granada) & BETMAn (by Vogel)

Expected outcomes from the meeting

- Determine the main quantities and supplemental data/information needed to be compiled in EXFOR
- Discuss the most appropriate format for compilation of thermal scattering data
- Discuss important/specific characteristics of measurements at the thermal and sub-thermal energies
- Prepare guidelines for compilation
- Receive a feedback from users
- Collect information/data.

Both double differential and total cross-sections can be used to benchmark thermal scattering evaluations.

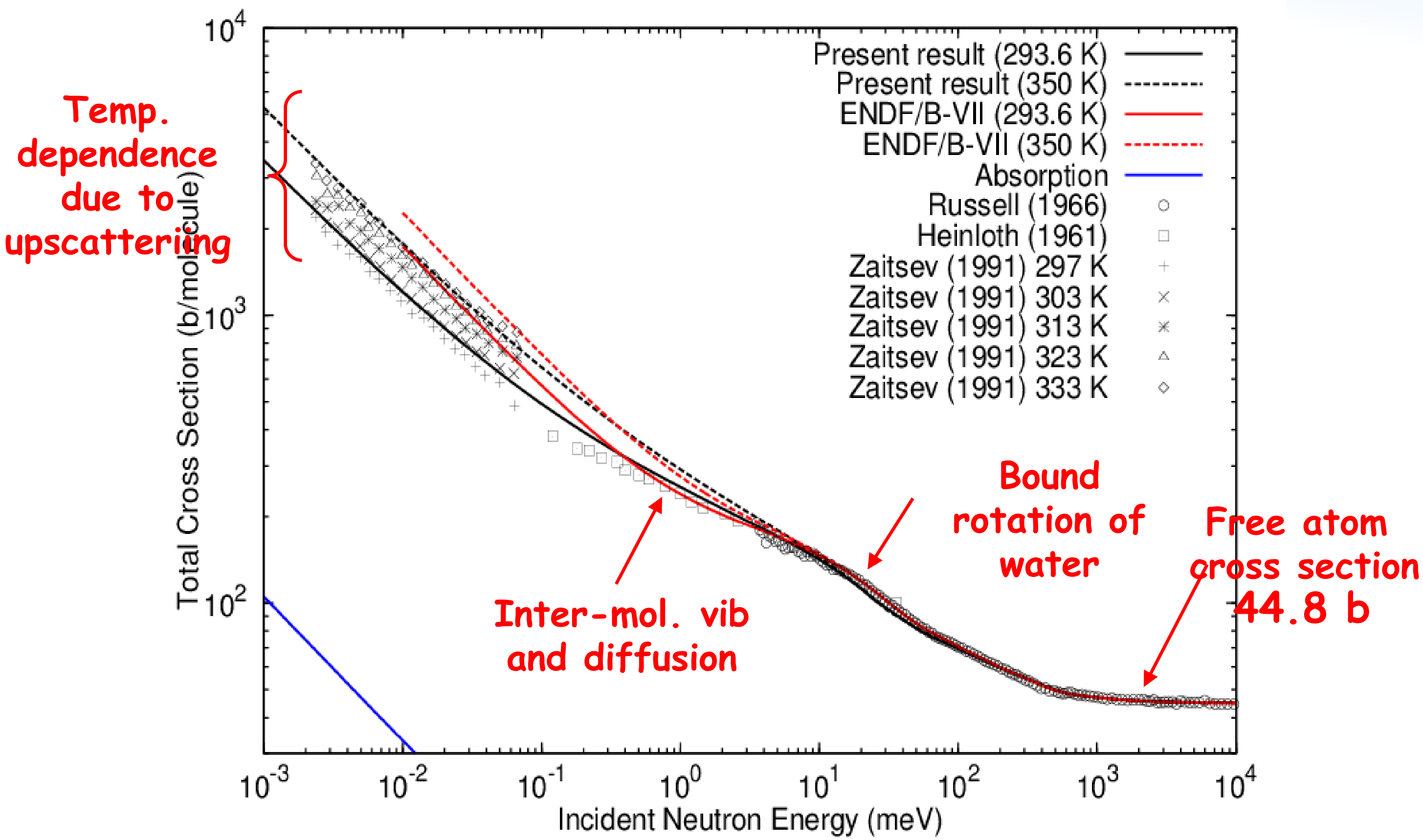
Total cross sections are not always sufficient, but necessary. They are cost efficient and with better statistics.



- The neutron energy is determined by means of the **time-of-flight technique**.
- **Sample-in sample-out** technique
- Measured spectra are **normalized** using the integral counts from a monitoring
- **Background** is measured and subtracted from both the incident and the
- transmitted beam spectra.
- Spectra are corrected by **dead time effects** from detectors and electronics

$$T_{exp} = N \frac{C'_{in} - B'_{in}}{C'_{out} - B'_{out}} \qquad \sigma(E) = \frac{-ln(T)}{N\Delta x}$$

Total cross-section for water



CF. Yoshiaki Kiyanagi CM EXFOR compilation of TSL

Neutron properties

Quantity	Particle	Wave
Wave length		$\lambda = \frac{h}{m \cdot v}$
Wave number		$k = \frac{2\pi}{\lambda}$
Momentum	$\vec{p} = m \cdot \vec{v}$	$\vec{p} = \frac{h \cdot \vec{k}}{2\pi} = \hbar \cdot \vec{k}$
Energy	$E = \frac{m}{2} v^2$	$E = \frac{h^2}{2m\lambda^2} = \frac{\hbar^2 \cdot k^2}{2m}$
Magnetic momentum μ_n	-1.913043 nuclear magnetons	
Spin S	1/2	

The wavelength of the thermal neutrons is of the same order of magnitude as the interatomic distances in solids and exceeds the nuclear radius. As a result:

- We consider that the nucleus is fixed and the scattering is elastic.
- Inelastic scattering occurs when an atom is displaced from its equilibrium position and due to the strong binding forces waves of atomic displacements are propagated throughout entire crystals.

Magnetic scattering occurs in materials that contain unpaired electrons.

Wave-particle relationships

	E (meV)	v (km/sec)	λ (Å)	k (Å^{-1})	f (cm^{-1})	T (K)	ω (THz)
Energy E of 1 meV	1	0.437	9.045	0.695	8.066	11.60	1.519
Velocity v of 1 km/sec	5.227	1	3.956	1.588	42.16	60.66	7.948
Wavelength λ of 1 Å	81.81	3.956	1	6.283	659.8	949.3	124.3
Wave vector k of 1 Å^{-1}	2.072	0.629	6.283	1	16.71	24.04	3.148
Optical frequency f of 1 cm^{-1}	0.124	0.154	25.69	0.245	1	1.439	0.188
Temperature T of 1 K	0.086	0.128	30.81	0.204	0.695	1	0.131
Angular frequency ω of 1 THz	0.658	0.354	11.15	0.564	5.31	7.63	1

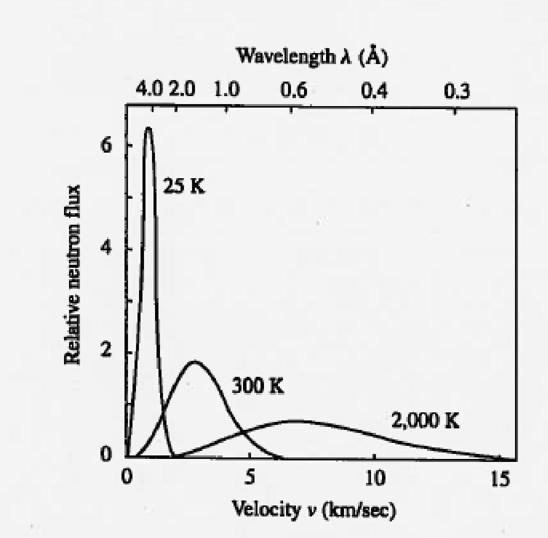
$$E = 5.227v^2 = 81.81/\lambda^2 = 2.0723k^2 = 0.1239f = 0.0861T = 0.568\omega$$

Characteristics of the main types of neutron energy distributions

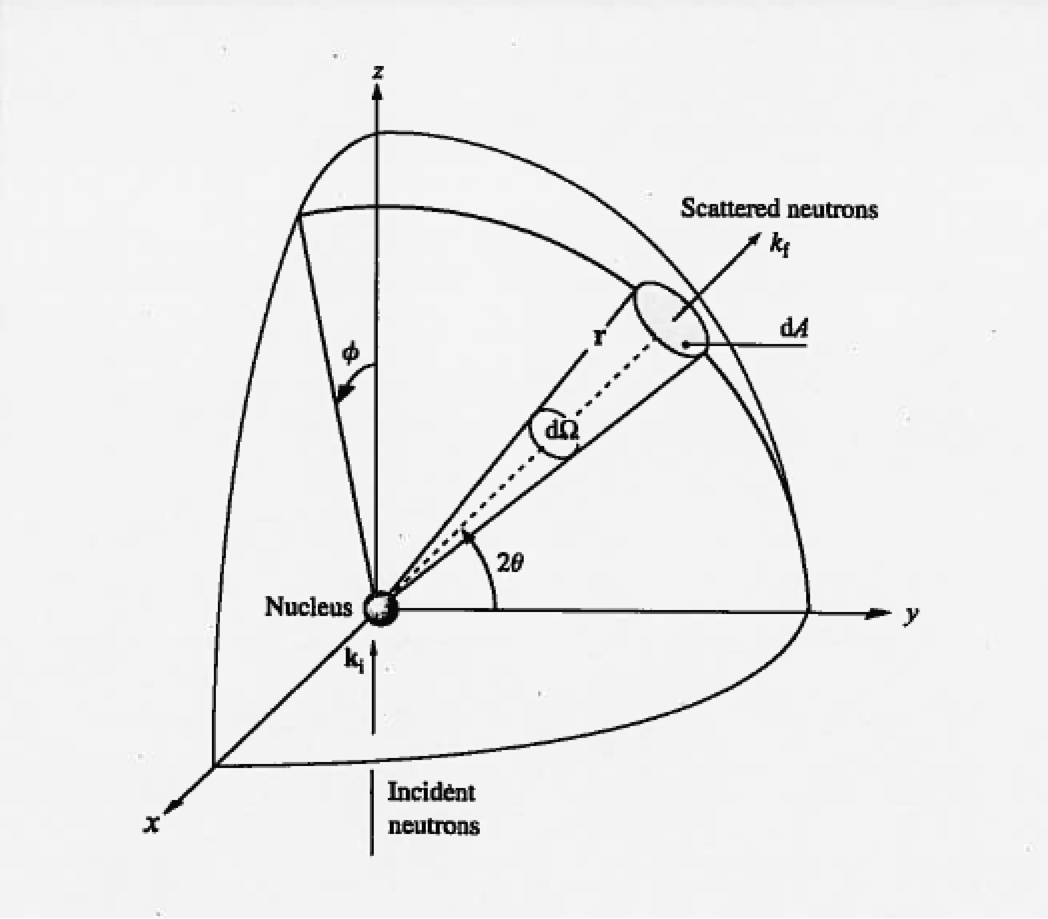
	Ultracold	Cold	Thermal	Epithermal	Fast
Energy	0.25 μeV	1 meV	25 meV	1 eV	2 MeV
Temperature	3 mK	12 K	290 K	12000 K	2.32×10^{10} K
Wave length	570 Å	9 Å	1.8 Å	0.29 Å	2.03×10^{-4} Å
Velocity	6.9 m/sec	440 m/sec	2200 m/sec	14000 m/sec	10^{7} m/sec

The energy of the fast neutrons produced by a reactor or an accelerator are reduced to:

- thermal region by moderator typically water or liquid hydrogen (low mass, large scattering cross section and low absorption cross section)
- cold neutrons by cold moderator of liquid hydrogen at 20 K
- short wavelengths, down to 0.3 Å can be produced by hot graphite moderator at temperature 2000K



Geometry of neutron scattering experiment



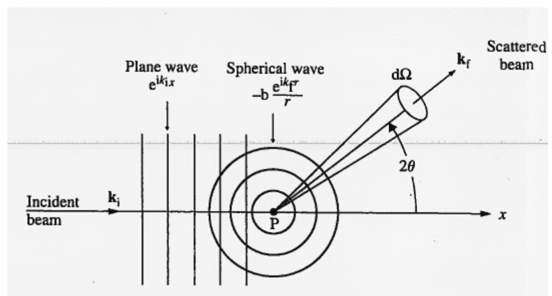
Scattering of a plane wave neutrons by a single (fixed) nucleus.

For thermal neutrons:

- Range of nuclear forces << neutron wavelength
- S-wave scattering
- Isotropic
- Elastic(energy of the neutron is too small to change the energy of the nucleus)

Incident wave function

$$\psi_i = e^{ikz}$$



Scattered beam

$$\psi_f = -b\frac{e^{ikz}}{r}$$

Density of 1 neutron per unit volume throughout all space $|\psi_i|^2 = 1$

I_0= neutron density x velocity = v

$I_f = \left|\psi_f\right|^2$ x velocity = $(b^2/r^2)\ v$

No. scatter neutrons = I_f x area =

$$\left(\frac{b^2}{r^2}\right) v \cdot 4\pi r^2 = (4\pi b^2)v$$

$$\sigma_{tot} = \frac{I_f}{I_0} = 4\pi b^2$$

b – scattering length (determined experimentally for each kind of nucleus)

Free and bound atoms scattering length

- The isotropic scattering, respectively the total scattering cross section, will depend on whether the nuclei are fixed or free to recoil during the scattering process.
- The scattering length measured in the laboratory-fixed frame is smaller by a factor (A/A+1) if the nucleus is free to recoil.
- It is conventional to quote the corresponding "bound-atom" values for scattering lengths and cross sections.

Scattering length characteristics

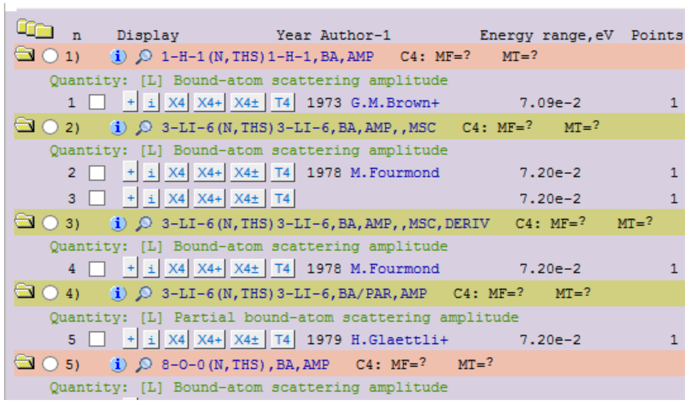
- *b* is a constant.
- *b* is a complex number. (In case absorption occurs in the interaction as well complex interaction potential is used, which gives complex scattering length. The imaginary part is related to the absorption cross section $b'' = \sigma_a/(2\lambda)$)
- when *b* is positive the potential V(r) is repulsive
- *b* is negative in some cases.
- *b* currently cannot be theoretically predicted and is determined experimentally for each nucleus.
- *b* varies erratically as a function of Z.

EXFOR compilation of scattering length for total scattering


```
DICTION          32     201605 Parameters (REACTION SF 6)        3000003200001
        ============================================================3000003200002
        General use                                              3000003200003
        ============================================================3000003200004
AMP        Scattering amplitude                                  3000003200009
```

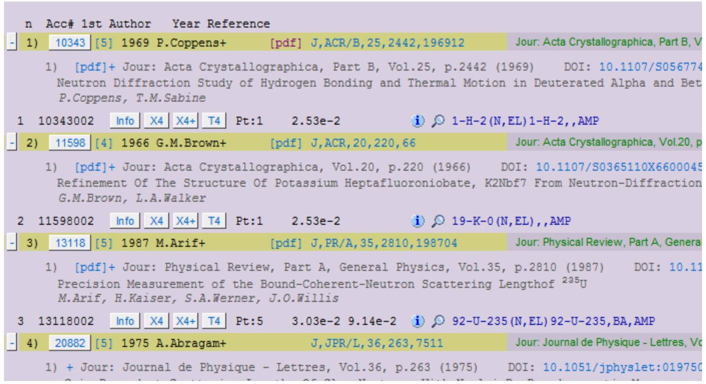
SF3 = THS

H-1, Li-6, O-0, Al-27, Cu-0, Sm-0, Sm-149



SF3 = EL

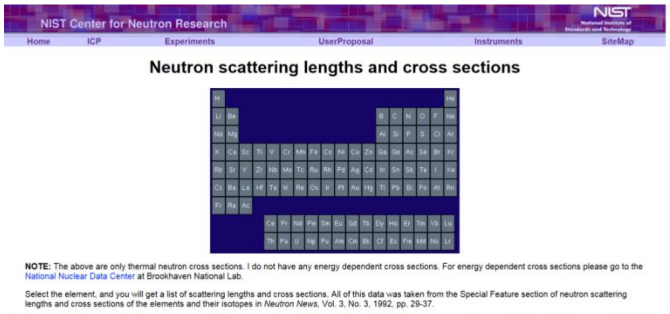
H-2, F-19, K-0, Bi-209, U-235

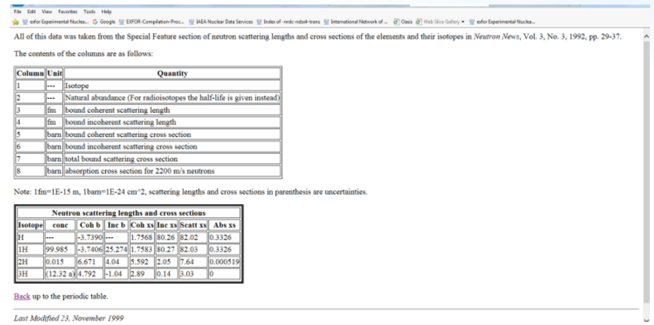


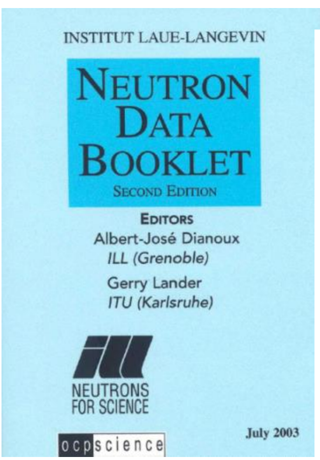
1. SF3 = THS is recommended EL – free atom scattering.
2. Completeness checking

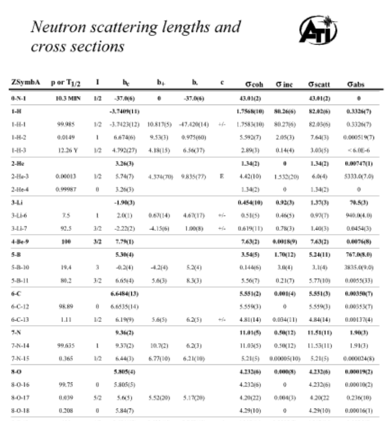
Thermal scattering length compilations

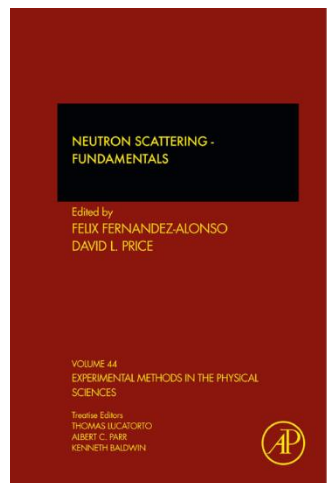
http://www.ncnr.nist.gov/resources/n-lengths/

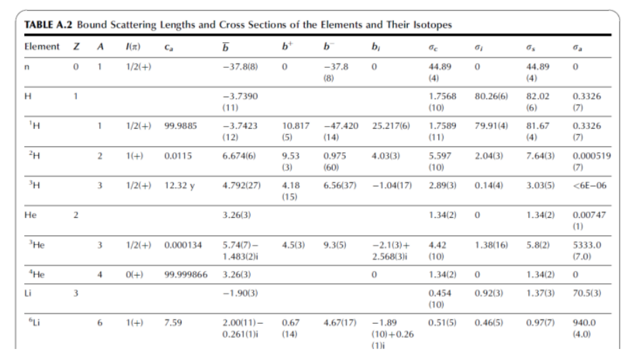












Double differential cross-section

	Initial state	Final state
Neutron	k Ψ_k	k' $\Psi_{k'}$
Scattering system	λ X_λ	λ' $X_{\lambda'}$

The differential cross section represents the sum of all processes in which the state of the scattering system changes from *λ* to *λ* ' , and the state of the neutron changes from **k** to **k'**

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{1}{\Phi}\frac{1}{d\Omega}\sum_{\substack{k' \\ E\ d\Omega}} W_{k,\lambda\to k'\lambda'}$$

where is the number of transitions per second from the state {**k**, *λ*} to the state {**k'** , *λ*' }, and Φ is the incident neutron flux.

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According to Fermi Golden Rule:

$$\sum_{\substack{k' \\ E\ d\Omega}} W_{k,\lambda\to k',\lambda'} = \frac{2\pi}{\hbar}\rho_{k'}|\langle k'\lambda'|V|k,\lambda\rangle|^2$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle k'\lambda'|V|k,\lambda\rangle|^2$$

$$E_\lambda + E = E_{\lambda'} + E'$$

$$\left(\frac{d^2\sigma}{d\Omega \mathrm{d}E'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 |\langle k'\lambda'|V|k,\lambda\rangle|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega)$$

It gives the possibility that the scattering changes the energy of the system by amount of

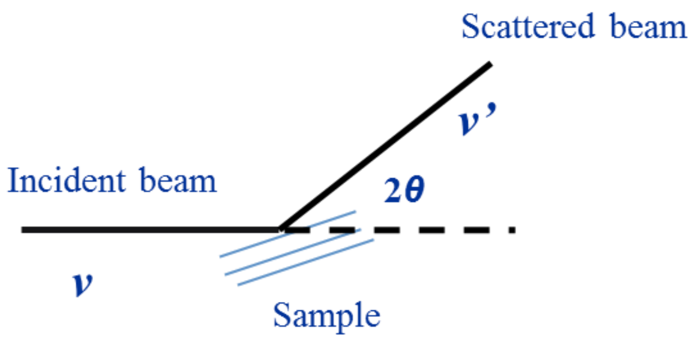
$\hbar\omega = E - E' = \frac{\hbar^2}{2m_n}\left(k^2 - k'^2\right)$: energy transfer

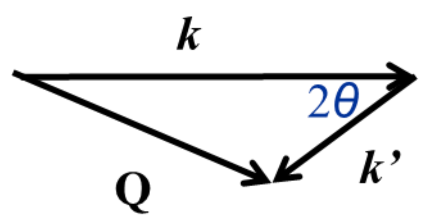
•

The energy ($\hbar\omega$) and momentum (Q) transfer are the basic characteristics of the thermal neutron scattering. The probability of scattering as a function of the variables (Q, ω) is a property of the particular sample and its environment (temperature, pressure, magnetic field, etc.)
Both energy and momentum of the interacting neutron and the sample obey the conservation low

$$\hbar\omega = E - E' = \frac{\hbar^2}{2m_n}\left(k^2 - k'^2\right) : \text{energy transfer}$$

$$Q^2 = k^2 + k'^2 - 2kk' \cos 2\theta$$





The interaction potential between the neutron a system of nuclei is a sum of interaction potentials with individual nuclei $V_j(r\text{-}R_j)$

$$V(r) = \sum_j V_j(r - R_j)$$

In general, the scattering of a neutron by a single bound nucleus is described within the Born approximation by the Fermi pseudopotential

$$V_j(r - R_j) = \frac{2\pi\hbar^2}{m} b_j \delta(r - R_j)$$

b_j is the scattering length of the j^{th} nucleus

Fourier transformation: $V(Q) = \frac{2\pi\hbar^2}{m} \sum_j b_j$

Where $\hbar Q = \hbar(k - k')$

The double differential cross section in the time domain

Although the scattering is described by the characteristics of the system in initial and final states without time dependence its evaluation becomes more transparent if we consider the explicit time evolution of particle positions $\mathbf{R}_j$

$$\delta(E_\lambda - E_{\lambda'} + \hbar\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} exp\left(i\,\frac{E_{\lambda'} - E_\lambda}{\hbar}\right) exp(-i\omega t)\mathrm{d}t$$

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{\lambda\to\lambda'} = \frac{k'}{k}\sum_{j,j'} b_{j'}^* b_j \langle\lambda'|exp(-iQ\cdot R_{j'})|\lambda\rangle \langle\lambda'|exp(iQ\cdot R_j)|\lambda\rangle$$

$$\times \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} exp\left(i\,\frac{E_{\lambda'}-E_\lambda}{\hbar}\right) exp(-i\omega t)\mathrm{d}t$$

In a real case, we have to sum all the final states keeping the initial state fixed and then average over all initial states of the target.

$$\frac{d^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'} b_{j'}^* b_j \int_{-\infty}^{\infty}\langle exp\left(-iQ\cdot R_{j'}(0)\right) exp\left(iQ\cdot R_j(t)\right)\rangle\, exp(-i\omega t)\mathrm{d}t$$

This is the **master formula** and it is the basis for the interpretation of all neutron-scattering experiments.

$$\frac{d^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'} = \frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\overline{b_{j'}b_j}\int_{-\infty}^{\infty} exp(-i\omega t)X_{jj'}(t)\,\mathrm{d}t$$

$$\mathrm{X}_{jj'}(t) = \langle exp\left(-iQ\cdot R_{j'}(0)\right) exp\left(iQ\cdot R_j(t)\right)\rangle$$

Each scatterer has its own *b* depending on the specific isotope, nuclear spin, etc.

$$\overline{b_j b_{j'}} = \bar{b}^2 \qquad j' \neq j$$

$$\overline{b_j b_{j'}} = \overline{b^2} \qquad j' = j$$

Coherent scattering

$$\left(\frac{d^2\sigma}{\mathrm{d}\Omega\,\mathrm{d}E'}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j,j'}\int_{-\infty}^{\infty} exp(-i\omega t)X_{jj'}(t)\,\mathrm{d}t \qquad \sigma_{coh} = 4\pi\bar{b}^2$$

Incoherent scattering

$$\left(\frac{d^2\sigma}{\mathrm{d}\Omega \mathrm{d}E'}\right)_{inc} = \frac{\sigma_{inc}}{4\pi}\frac{k'}{k}\frac{1}{2\pi\hbar}\sum_{j}\int_{-\infty}^{\infty} exp(-i\omega t)X_j(t)\,\mathrm{d}t \qquad \sigma_{inc} = 4\pi\left(\overline{b^2} - \bar{b}^2\right)$$

Information about the neutron

Information about the scattering system

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi}\frac{k'}{k}N(\sigma_{coh}S_{coh}(Q,\omega) + \sigma_{inc}S_{inc}(Q,\omega))$$

$\boldsymbol{S(Q,\omega)}$ scattering function of the system. It gives probability that the scattering changes the energy of the system by amount of $\hbar\omega = E - E'$ and its momentum by $\hbar Q = \hbar(k-k')$

$S_{coh}(Q,\omega)$ and $S_{inc}(Q,\omega)$ are the coherent and incoherent scattering laws.

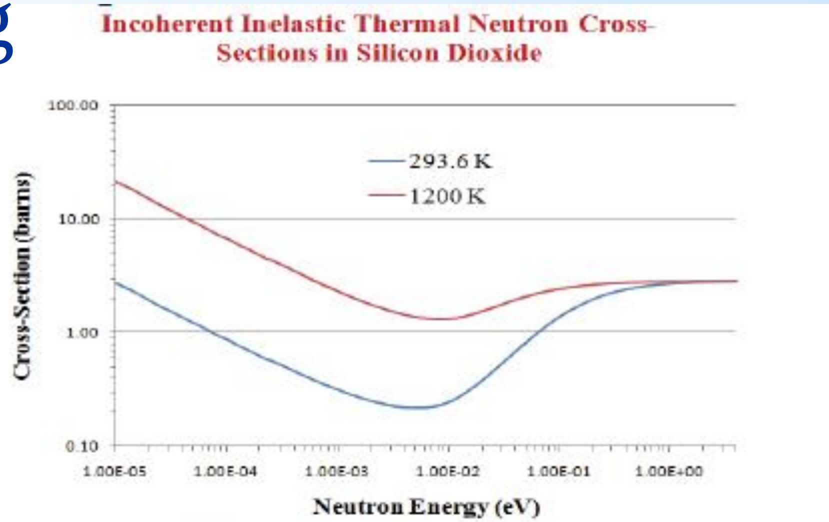
$$S_{coh}(Q,\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} exp(-i\omega t)X_{coh}(Q,t)\,\mathrm{d}t \qquad S_{coh}(Q,\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} exp(-i\omega t)X_{coh}(Q,t)\,\mathrm{d}t$$

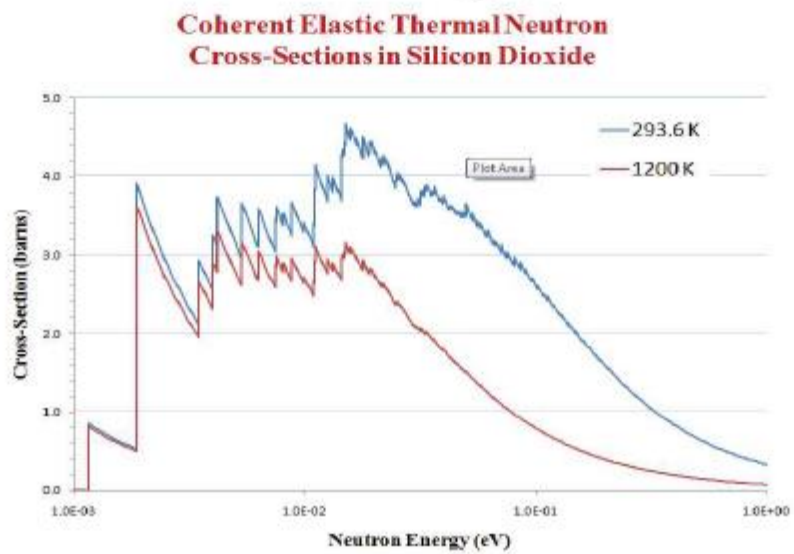
The Fourier transform are called Intermediate Scattering Functions

$$\chi_{coh}(Q,t) = \frac{1}{N}\sum_{j,j'}\langle exp\left(-iQ\cdot R_{j'}(0)\right) exp\left(iQ\cdot R_j(t)\right)\rangle \qquad \chi_{inc}(Q,t) = \frac{1}{N}\sum_{j}\langle exp\left(-iQ\cdot R_{j}(0)\right) exp\left(iQ\cdot R_j(t)\right)\rangle$$

These correlation functions, scattering laws and intermediate scattering functions contain all the information on the structure and dynamics of the scattering system. This information is obtained in a direct way in the measurement of the double differential scattering cross section.

Comparison between coherent and incoherent scattering





A lattice which has only one atom in the unit cell is called **Bravais lattice.** The central position is determined by I_j. Considering the thermal motion the j^{th} atom position is determined by $R_j = I_j + u_j$, with u_j the displacement from the I_j.

Coherent scattering:

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)_{coh} = \frac{\sigma_{coh}}{4\pi}\frac{k'}{k}\frac{N}{2\pi\hbar}\exp\langle U^2\rangle\sum\exp(i\boldsymbol{\kappa}\cdot\mathbf{l})\int_{-\infty}^{\infty}\exp\langle UV\rangle\exp(-i\omega t)dt$$

Debye Waller Factor: related to the mean-square displacement of each atom around its equilibribum position. depends on the temperature

Related to the creation of phonons. No phonon creation for elastic scattering

$|\mathrm{k}| = |\mathrm{k}'|$

Coherent elastic scattering is so called Brag scattering

Mean-square displacements are associated to the oscillation modes. Since the number of degrees of freedom is close to 10^{23}, oscillation modes are expressed as an integral over all the frequencies by means of the density of states $Z(\omega)$ (or frequency spectra)

Inelastic scattering experiments

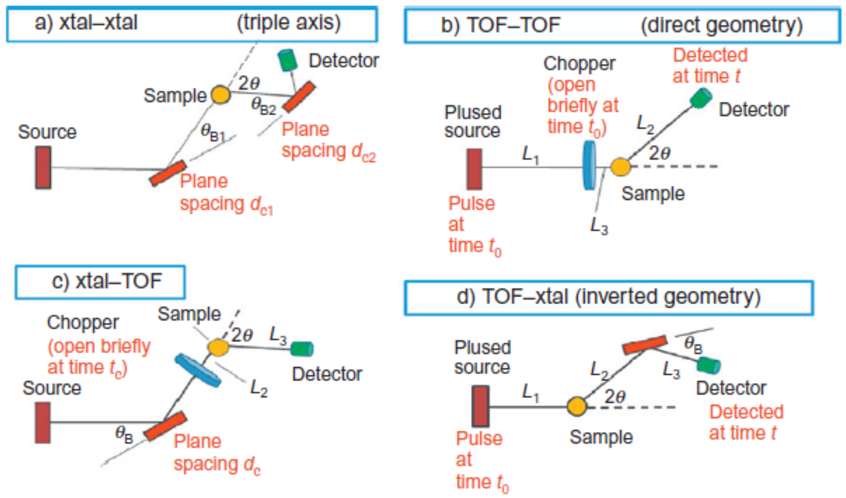


FIGURE 3.2 Typical inelastic scattering techniques.

An inelastic scattering experiment involves the determination of the magnitudes of $\mathbf{k}_i$ and $\mathbf{k}_f$ and the scattering angle Φ for each detected neutrons.

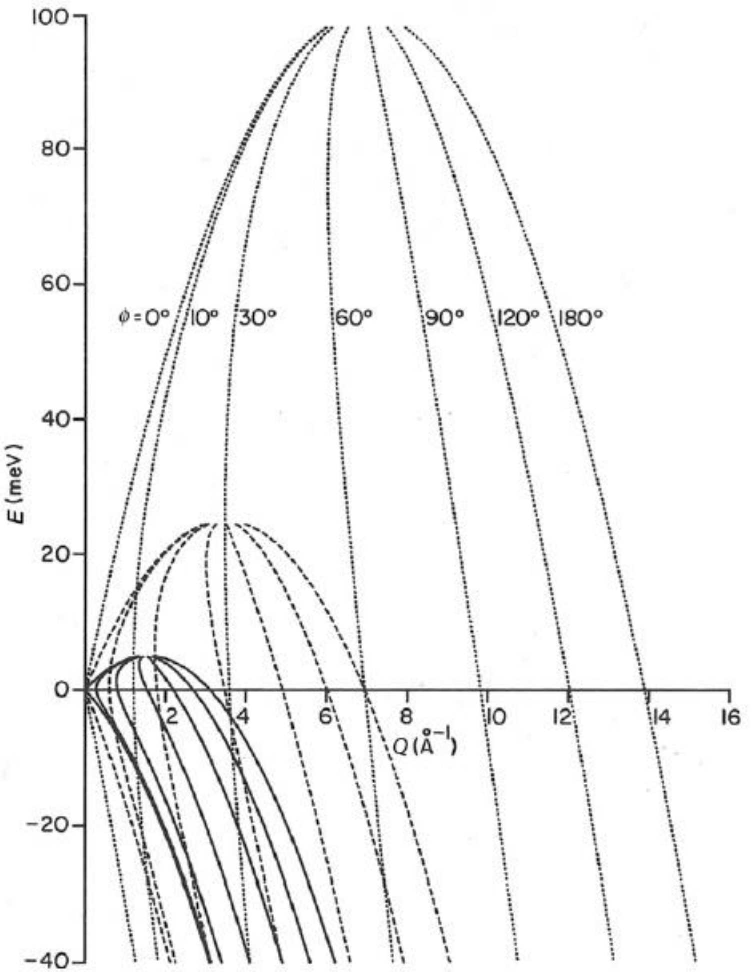


FIGURE 1.6 Relationship between energy transfer E and wave vector Q for three different incident energies $E_i = 5$ meV (solid curves), 25 meV (dashed curves), and 100 meV (dotted curves). For each E_i, loci are shown for different values of the scattering angle ϕ.

The dynamic structure factor can directly be extracted from the measured scattered intensity

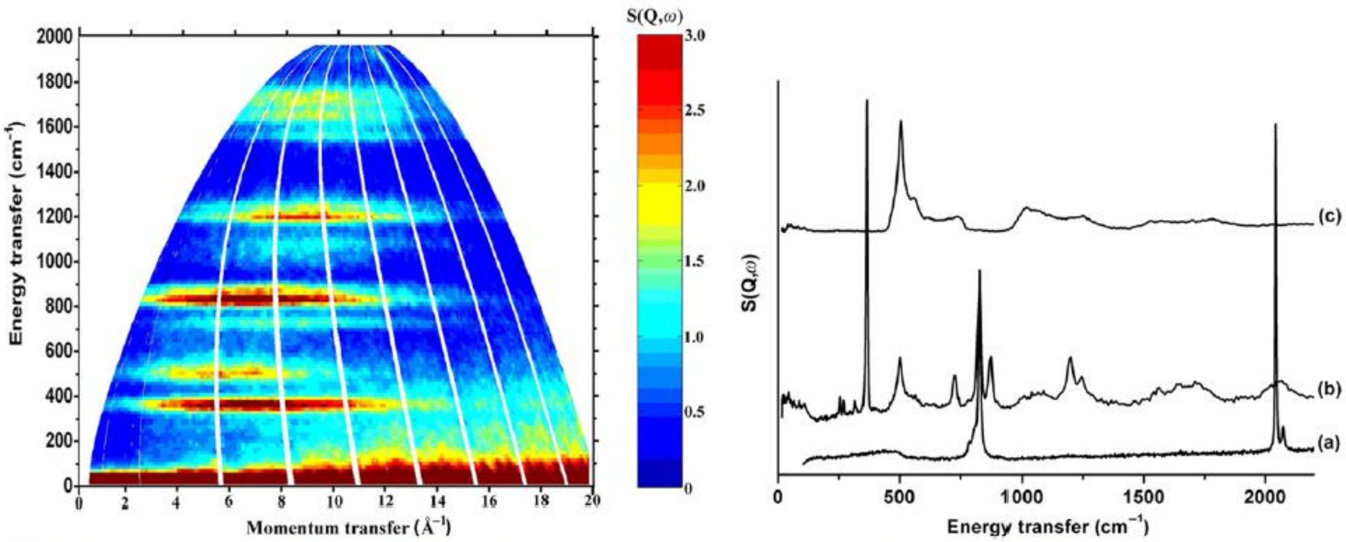


FIGURE 1.10 The contour color plot on the left shows inelastic neutron-scattering data for the metal-hydride complex Rb_2PtH_6 using an incident neutron energy of 2000 cm^{-1} (~250 meV). The figure on the right compares vibrational spectra using (a) Raman scattering and (b) inelastic neutron scattering along the proton-recoil line for the same compound. The top trace (c) corresponds to the inelastic neutron-scattering response from the reference material RbH, also present as a reaction by-product in (b). The broad energy features in the Raman data below ca. 500 cm^{-1} arise from fluorescence backgrounds. *Reprinted with permission from Ref. [80].*

- EXFOR format allows compilation of energy and momentum transfer as independent variables.
- If the dynamical structure factor is compile SF8=RAW need to be compiled.

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi}\frac{k'}{k} N(\sigma_{coh} S_{coh}(Q,\omega) + \sigma_{inc} S_{inc}(Q,\omega))$$

NJOY Nuclear Data Processing System generates scattering laws and cross sections for different materials at different temperatures.

Input parameters
(discrete and continuous phonon spectrum, diffusion component ...)

→

LEAPR module of NJOY

→

TSL data in ENDF-6 format
MF=7

$$S(\alpha,\beta) = k_B T exp\left(\frac{-\hbar\omega}{2k_B T}\right) S(q,\omega)$$

$$\alpha = \frac{q^2\hbar^2}{2Mk_B T} = \frac{E_i + E_f - 2\mu\sqrt{E_i E_f}}{Ak_B T}$$

$$\beta = \frac{-\hbar\omega}{k_B T} = \frac{E_i - E_f}{k_B T}$$

Outcomes

- The EXFOR coverage for neutron induced cross sections data at thermal incident energies should be improved;
- The importance and the needs of the nuclear data should be emphasised in order support the ND community in their applications for beam time at the large scattering facilities;
- The procedures for analysis of the scattering cross section measurement were discussed;
- Evaluation methods for TSL evaluations in connection with recent requests for improved scattering data were reviewed;
- The descriptions of the thermal scattering quantities in the EXFOR compilation manual LEXFOR were revised;
- the physics of thermal scattering, and its differences from analysis of scattering in epithermal range was summarized;
- A template with required experimental information to be compiled was assembled;
- A list of materials relevant to nuclear applications to be considered for EXFOR compilation was provided in order to guide NRDC community to select relevant materials.

Recommendations

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- Double differential cross section, differential cross section, and total cross section experimental data should be stored and details of the experiments and instruments shall be laid out clearly.
- Publish guidelines for what is needed for acceptable submissions to EXFOR (specify needed/suggested metadata including experimental details needed to understand the processing of the data). This should be provided as template for EXFOR data compilers.
- $S(q,\omega)$ or $S(\alpha, \beta)$ could be stored in a new dedicated section of EXFOR with details of the derivation being provided.
- Phonon spectrum, structural parameters, and other information derived from neutron double differential scattering experiments, X-ray crystallography and modelling should be stored in a separate repository accessible to the evaluators as derived data, with details of the derivation being provided.

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Thank you!