WP2016-08

LEXFOR "Thermal Neutron Scattering"

(N. Otsuka, V. Semkova, 2016-05-06, Memo 4C-3/403)

We prepared a revised LEXFOR chapter "Thermal Neutron Scattering", and it was further reviewed and revised in the Consultant Meeting on the "EXFOR Compilation of Thermal Neutron Scattering Data" (2-4 November 2015, see also INDC(NDS)-0697) with experts of this field. We do not often deal with this subject during compilation, and we wish the revised version will be a good introduction to EXFOR compilers.

Thermal Neutron Scattering

Theory

The scattering of slow neutrons (energies less than the chemical binding energy, and not close to resonance region, typically less than a few eV), with matter depends on the atomic structure of the material (because the wavelength of slow neutrons is of the order of inter-atomic distances) and on the atomic dynamics in the scattering medium (because the energy of slow neutrons is of the same order as the energy of thermal motion of atoms in crystals and solids). Van Hove formulated the double differential cross sections considering the structure and dynamics as

$$d^2\sigma/d\Omega dE' = (1/2\pi\hbar)\,(k'/k)\,\Sigma_{ij}\, b_i b_j \int_{-\infty}^{+\infty} dt \langle \exp(-i\mathbf{q}\cdot\mathbf{r}_j(0))\exp(-i\mathbf{q}\cdot\mathbf{r}_i(t))\rangle_T \exp(-i\omega t)$$

where k and k' are the initial and final wave numbers of the neutron, b_i is the scattering length of the nucleus i which is at position $\mathbf{r}_i$ at time t,$\mathbf{q}=\mathbf{k'}-\mathbf{k}$ is the momentum transfer of neutron, and $\hbar\omega=E'-E$ is the energy transfer of neutron. $\langle ... \rangle_T$ denotes averaging over the canonical ensemble characterized by the temperature T. If we denotes the integral by $S_{ij}(\mathbf{q},\omega)$, and decompose the differential cross section to the $i\neq j$ and $i=j$ part:

$$d\sigma/d\Omega dE' = (1/2\pi\hbar)\,(k'/k)\,[\langle b\rangle^2\Sigma_{i\neq j}\, S_{ij}(\mathbf{q},\omega) + \langle b^2\rangle\Sigma_{i=j}\, S_{ij}(\mathbf{q},\omega)]$$

$$= (1/2\pi\hbar)\,(k'/k)\,[\langle b\rangle^2\Sigma_{i,j}\, S_{ij}(\mathbf{q},\omega) + (\langle b^2\rangle - \langle b\rangle^2)\Sigma_{i=j}\, S_{ij}(\mathbf{q},\omega)]$$

where $\langle b\rangle^2$ is $\langle b_i b_j\rangle$ with $i\neq j$ and $\langle b^2\rangle=\langle b_i b_j\rangle$ with i=j. The first term of the second equation involving all nuclear states (isotopes and spin states of the compound) describes **coherent scattering** while the second term involving a single nuclear state describes **incoherent scattering**.

Coding

- For all scattering processes where molecular and crystalline forces are involved the code `THS` is used in reaction SF3. For other processes (e.g., total), the modifier `TMP` is added for temperature different from the room temperature to indicate that the quantity is temperature dependent.

- When the compiler is aware that the quantity depends on the orientation of the sample (e.g., transmission for a single crystal), it must be indicated by SF8=`MSC` with free text.
- The sample temperature is given under the heading `TEMP`.
- The crystal structure of the sample is given under the keyword `SAMPLE`.

Coherent and incoherent scattering length

The quantities $b_{coh}=\langle b\rangle$ and $b_{inc}= (\langle b^2\rangle-\langle b\rangle^2)^{1/2}$ are known as the coherent and incoherent scattering length.

The scattering length for a **free atom** (mass number A) is a factor A/(A+1) smaller than that for a **bound atom**. Their distinction is important for light nuclides.

Some strong neutron absorbers (e.g., ^{113}Cd, ^{157}Gd) may have an imaginary part of the scattering length. The imaginary part of $\langle b\rangle$ is related with the absorption cross section by $\mathrm{Im}(\langle b\rangle)=k\sigma_{abs}(E)/4\pi$ (optical theorem) at $E\rightarrow 0$.

The scattering length b is related with the **scattering amplitude** f(E) by $b=-\lim_{E\rightarrow 0}f(E)$. (Sometimes scattering length is called as scattering amplitude.)

REACTION Coding: `COH` or `INC` in SF5 and `AMP` in SF6. `IM` in SF5 for imaginary part.

Examples:

`(6-C-12(N,THS)6-C-12,BA/COH,AMP)`
Bound atom coherent scattering length of ^{12}C

`(23-V-51(N,THS)23-V-51,FA/INC,AMP)`
Free atom incoherent scattering length of ^{51}V

`(64-GD-157(N,THS)64-GD-157,COH/IM,AMP)`
Imaginary part of coherent scattering length of ^{157}Gd

Contribution of potential scattering and resonance scattering

The bound atom scattering length is the sum of the contribution from potential scattering and all s-wave resonances:

$$[A/(A+1)]|b_{\pm}| = R' - [(A+1)/A]\ [\hbar/(8m)^{1/2}]\ \Sigma_{i\pm}\,[(\Gamma_{n,i}/E_{0,i}^{3/2}) - i\,(\Gamma_{n,i}\Gamma_n/2E_{0,i}^{5/2})],$$

where m is the neutron mass and $\hbar c/(8m)^{1/2}\sim 2277$ fm eV$^{1/2}$. R' is the **potential scattering radius**, A is the mass number of the nuclei, $\Gamma_{n,i}$ and Γ_i are the neutron and total width of the i-the resonance at the resonance energy $E_{0,i}$. $\Sigma_{\pm}$ means summation for all resonance having the same spin $J_+=I+1/2$ or $J_+=I-1/2$. Their weighted mean gives $\langle b\rangle=g_+b_++g_-b_-$ with $g_{\pm}=[2(I\pm 1/2)+1]/[(2I+1)2]$, where I is the spin of the target nucleus

Note that only J=I+1/2 is possible for spin zero nuclei, and $b_{coh}=b_+$ and $b_{inc}=0$ for them. For example, thorium gives no incoherent scattering because it is enriched to thorium-232 and its ground state spin is zero.

Coherent and incoherent scattering cross section

The quantities $\sigma_{coh}=4\pi b_{coh}^2$ and $\sigma_{inc}=4\pi b_{inc}^2$ are known as the coherent and incoherent scattering cross section. Their values for bound and free atom are related by the factor A/(A+1). Their sum $4\pi(b_{coh}^2+b_{inc}^2)$ gives the total scattering cross section of fixed nuclei.

Examples:

`(6-C-12(N,THS)6-C-12,BA/COH,SIG)`

Bound atom coherent cross section of ^{12}C

`(23-V-51(N,THS)23-V-51,INC,SIG)`

Incoherent cross section of ^{51}V

References

[1.] S. Mughabghab, Atlas of neutron resonances: Resonance parameters and thermal cross sections Z=1-100 (Elsevier, 2006).

[2.] B.T.M. Willis and C.J.Carlile, Experimental neutron scattering (Oxford University Press, London, 2009).

[3] ILL Neutron Data Booklet, Editors Albert-José Dianoux and Gerry Lander (2003 Institute Laue-Langevin, France)