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The ENDF-6 file 7 and its possible evolutions with respect to the processing needs

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Summary

Position of the problem

Some proposals for thermal binding data in the ENDF format

Conclusion

Micellaneous

Free Gas Model

Free Gas (FG) is the most widely used model to perform the Doppler broadening (DB) of the cross sections and to calculate the double differential scattering cross section.

At the processing step, the user can choose freely :

1. the temperatures of the medium,
2. the incident neutron energy ranges and the associated modelling of the thermal agitation(*),
3. to take into account or not the resonant(**) character of the scatterer.

(*) A similar idea has been presented by David Brown, during the last WG42 meeting, speaking of metadata associated to TS data.

(**) see papers of Blackshaw and Murray NSE (1967) ; Richard Sanchez [NSE (1991), Annals of Nucl. Energy (2016)] about the free gas Doppler Broadening Kernel (DBK).

Thermal binding Model

ENDF Thermal Scattering (TS) evaluation file 7 allows to calculate the double differential scattering cross section.

The user cannot choose freely :

1. the temperatures of the medium,
2. the incident neutron energy ranges and the associated modelling of the thermal agitation (Perhaps yes, need clarification).
3. to take into account the resonant character of the scatterer (constant free scattering cross section imposed but scattering law seems basically a property of the condensed matter),

ENDF-6 TS data

Temperatures of the medium

$S(\alpha, \beta)$, as stated in the ENDF format manual, should not be interpolated in temperature but no rule of interpolation is given for inelastic incoherent cross section.

The user can use any interpolation scheme without means to check it.

The coherent elastic and incoherent elastic scattering cross sections have interpolation specifications in the ENDF format manual.

A user has no mean to choose the temperatures of the medium at the processing step.

Incident Neutron Energy Ranges

Free Gas Model

How the incident neutron energy ranges are sliced in term of thermal agitation modelling is not formally defined in ENDF. It is decided at the processing level.

For the FG model, we have a clear picture of the degree of validity of each model versus the incident neutron range.

Using the Free Gas model, we can do the following modelling by increasing incident neutron energy :

1. free gas model used for the calculation of the cross sections (DB) and the scattering angle-energy distribution (DBK),
2. free gas model used only for the calculation of the cross sections (DB) and the static model (or non resonant FG) used for the calculation of the angle-energy distribution,
3. static model used for the calculation of the cross sections and the scattering angle-energy distribution (no thermal motion, purely nuclear).

Incident Neutron Energy Ranges (cont'd)

Thermal binding model

Using the thermal binding model, we would like to do similar modelling as the one done using the Free Gas Model but...

in the preamble of file 7 description we read : "File 7 contains neutron scattering data for the thermal neutron energy range ($E < 5eV$)".

The only data, more or less, related to the discussed matter are $\epsilon = E/T$ (E incident energy) and E_{max} (related to incident energy).

- ϵ describes the transition to the static model where the cross section tends to the free scattering cross section,
- E_{max} defines the boundary between the use of the tabulated $S(\alpha,\beta)$ and the SCT model (kind of free gas model with an effective temperature with a forcing of the detailed balance).

ENDF TS data

Doppler Broadening

The scattering law can be used in Doppler Broadening [Lamb in Phys. Rev. (1939) ; Nelkin- Parks in Phys. Rev. (1960) ; Jackson-Lynn in Phys. Rev. (1961) ; applied work of Naberejnev-Mounier-Sanchez in NSE (1999)].

In the preamble of file 7 description we read : "File 7 contains neutron scattering data for the thermal neutron energy range ($E < 5$ eV)".

Questions :

- Is it licite to use the scattering law for the Doppler Broadening, in particular, above 5 eV ?
- These authors propose to use Free Gas model with an effective temperature (weak binding approximation). It's very similar to the SCT approximation. Is it correct to use this approximation far above 5 eV for example ? Do we need the detailed balance forcing for the Doppler Broadening as in SCT or only FG with an effective temperature ?

ENDF-6 TS data

Secondary Scatterers

The allowed models for the secondary scatterers are, in ENDF order, the Short Collision Time (0), the Free Gas (1), and the Diffusive motion (2). The last one is not specified in ENDF format manual.

In the most recent TSL, Free Gas model is the only specified model in this context.

Some assertions or questions about the analytical laws for a secondary scatterer :

- Short Collision Time (SCT) should preferred over the free gas model because it is designed to replace $S(\alpha, \beta)$ at high energy. Is it as good as FG everywhere ?
- Diffusion motion is not proposed in replacement of scattering law at high energy. As it is proposed as analytical law for secondary scatterers ? Is it as good as the FG everywhere ?

LEAPR data

as ENDF data

The first evolution could be the introduction of the actual LEAPR input data as an additional way to specify TS data in ENDF, that is to say for example, the weighted phonon spectra and the crystallographic data with a temperature interpolation scheme.

The crystallographic data for coherent scattering are hard coded in LEAPR. For more versatility and reuse, ENDF data for coherent scattering could be the crystallographic structure, unit cell dimensions and the scattering length.

Using these basic data, the definition of covariance data is also more condensed. The basic data are probably highly correlated in temperature so covariances between scattering law at different temperatures can be expressed in a condensed form.

This proposal answers to the first need for the processing : the user must be able to choose the temperatures of the medium.

Thermal binding model

Using the ENDF thermal binding data, we would like to do the following modelling by increasing incident neutron energy :

1. thermal binding model used for the calculation of the cross sections (DB) and the scattering angle-energy distribution (DBK),
2. thermal binding model (or SCT model) used for the calculation of the cross sections (DB) and the static model (or non resonant SCT model) used for the calculation of the scattering angle-energy distribution.

The proposal is to write in the ENDF format manual the necessary theoretical corpus enabling the user in the processing to switch properly between the thermal motion models. New ENDF format for thermal binding model should be enlarged to the problematic of the Doppler Broadening and the Doppler Broadening kernel (angle-energy distribution).

Conclusion

More fundamental data concerning the condensed matter in the ENDF format (including the problematic of the Doppler Broadening) should allow to the user, in the processing, to choose freely :

- the temperatures of the medium,
- the incident neutron energy ranges and the associated thermal motion models to switch smoothly among them,
- to take into account or not the resonant(*) character of the scatterer.

(*) The last item is connected to the Doppler Broadening Kernel (angle-energy distribution) in presence of chemical binding. It is not a trivial aspect [Word-Trammell in Phys. Rev. (1981) ; Naberejnev in Annals of Nucl. Energy (2001) ; Courcelle-Rowlands in arXiv (2007)]

ENDF-6 TS data

Free Scattering Cross Section

Free Scattering Cross Sections are specified in TS data.

But the thermal data are used with various nuclear data evaluation where scattering cross section (MT=2) may have different values at the same thermal energy. Perhaps it would be interesting to establish a connection with the resonances data (scattering radius, s-wave phase shift).

A possible mismatch in the scattering cross section may occur in the frontier between thermal and epithermal ranges.

ENDF-6 TS data

Natural element

Natural TS data exists for example Zr bound in ZrH.

Actually, in the processing, each isotope of Zr shares the same thermal data.

Is there a better processing for natural TS if only isotopes are available in nuclear data evaluation ?

Basic formulae

Doppler-broadened cross-section

$$\sigma_{s,T}(v) = \frac{1}{v} \int d\vec{V} M_T(V) v_r \sigma_{s,T=0}(v_r) \quad (1)$$

Doppler-broadened kernel

$$P_s(\vec{v}, E', \mu_L) = \frac{1}{v \sigma_s(v, T)} \int d\vec{V} M_T(V) v_r \sigma_{s,T=0}(v_r) \boxed{P(\vec{v}, \vec{V}, E', \mu_L)} \quad (2)$$

- $M_T(\vec{V})$: Maxwellian distribution of the target velocity,
- $\vec{v}_r = \vec{v} - \vec{V}$: relative speed between the neutron and the target,
- $\sigma_{s,T=0}$: scattering cross section at 0 Kelvin,
- $\boxed{P(\vec{v}, \vec{V}, E', \mu_L)}$: kernel of the two-body elastic scattering,
- \vec{v} and \vec{V} : incoming neutron and target velocities,
- E and E' : incident and outgoing neutron's energies,
- μ_L : deviation cosine of the neutron in LAB.