7. FILE 7. THERMAL NEUTRON SCATTERING LAW DATA

7.1. General Description

File 7 contains neutron scattering data for the thermal neutron energy range (E<5 eV) for moderating materials. Sections are provided for elastic (MT=2) and inelastic (MT=4) scattering. Starting with ENDF/B-VI, File 7 is complete in itself, and Files 3 and 4 are no longer required to obtain the total scattering cross section in the thermal energy range.

7.2. Coherent Elastic Scattering

The coherent elastic scattering from a powdered crystalline material may be represented as follows:

$$\frac{d^2\sigma}{dEd\Omega}(E \to E', \mu, T) = \frac{1}{E} \sum_{i=1}^{E_i<E} s_i(T)\delta(\mu - \mu_i)\delta(E - E')/2\pi \tag{7.1}$$

where

$$\mu_i = 1 - \frac{2E_i}{E} \tag{7.2}$$

In these formulas:

E = incident neutron energy (eV),
E′ = secondary neutron energy (eV),
μ = cosine of the scattering angle,
T = moderator temperature (K),
E_i = energies of the Bragg edges (eV),
s_i = proportional to the structure factors (eV-barns),
μ_i = characteristic scattering cosines for each set of lattice planes.

The Bragg edges and structure factors can be calculated from the properties of the crystal lattice and the scattering amplitudes for the various atoms in the unit cell.[1]

The quantity actually given in the file is

$$S(E,T) = \sum_{i=1}^{E_i<E} S_i(T) \tag{7.3}$$

which is conveniently represented as a stair-step function with breaks at the Bragg edges using histogram interpolation.

7.2.1. Formats for Coherent Elastic

The parameters to be used to calculate coherent elastic scattering are given in a section of File 7 with MT=2. The following quantities are defined:

ZA,AWR	Standard charge and mass parameters.
LTHR	Flag indicating which type of thermal data is being represented. LTHR=1 for coherent elastic scattering.
T_i	Temperature (K).

[1] As an example, the HEXSCAT code [Ref. 1] can be used for hexagonal lattices.

LT Flag for temperature dependence. The data for the first temperature are given in a TAB1 record. The data for subsequent temperatures are given in LIST records using the same independent variable grid as the TAB1 record.

LI Flag indicating how to interpolate between the previous temperature and current temperature. The values are the same as for INT in standard TAB1 records.

NR,E_{int} Standard TAB1 parameters. Use INT=1 (histogram).

NP Number of Bragg edges given.

The structure of a section is

```
[MAT, 7, 2/   ZA,  AWR, LTHR,  0,  0,  0] HEAD                LTHR=1
[MAT, 7, 2/    T0, 0.0,   LT,  0, NR, NP/ Eint / S(E,T0) ] TAB1
[MAT, 7, 2/    T1, 0.0,   LI,  0, NP,  0/ S(Ei,Ti) ] LIST
          --------------------------
          <repeat LIST for T2, T3, ...TLT+1>
          --------------------------
[MAT, 7, 0 /  0.0, 0.0,    0,  0,  0,  0] SEND
```

7.2.2. Procedures for Coherent Elastic

The coherent elastic scattering cross section is easily computed from S(E,T) by reconstructing an appropriate energy grid and dividing S by E at each point on the grid. A discontinuity should be supplied at each E_i, and log-log interpolation should be used between Bragg edges. The cross section is zero below the first Bragg edge.

The function S(E,T) should be defined up to 5 eV. When the Bragg edges get very close to each other (above 1 eV), the "stair steps" are small. It is permissible to group edges together in this region in order to reduce the number of steps given while still preserving the average value of the cross section. Either discrete-angle or Legendre representations of the angular dependence of coherent elastic scattering can be constructed. It is necessary to recover the values of $s_i(T)$ from S(E,T) by subtraction.

7.3. Incoherent Elastic Scattering

Elastic scattering can be treated in the incoherent approximation for partially ordered systems such as ZrH_x and polyethylene. The differential cross section is given by

$$\frac{d^2\sigma}{dE\,d\Omega}(E \to E', \mu, T) = \frac{\sigma_b}{4\pi} e^{-2EW'(T)(1-\mu)}\,\delta(\mu)\delta(E-E') \tag{7.4}$$

where

σ_b is the characteristic bound cross section (barns),

W' is the Debye-Waller integral divided by the atomic mass (eV^{-1}),

and all the other symbols have their previous meanings. The integrated cross section is easily obtained:

$$\sigma(E) = \frac{\sigma_b}{2}\left(\frac{1-e^{-4EW'}}{2EW'}\right) \tag{7.5}$$

Note that the limit of σ for small E is σ_b.

7.3.1. Format for Incoherent Elastic

The parameters for incoherent elastic scattering are also given in a section of File 7 with MT=2, because coherent and incoherent representations never occur together for a material. The following quantities are defined:

ZA,AWR	standard material charge and mass parameters.
LTHR	flag indicating which type of thermal data is being represented. LTHR=2 for incoherent elastic.
NP	number of temperatures.
SB	characteristic bound cross section (barns)
W′(T)	Debye-Waller integral divided by the atomic mass (eV^{-1}) as a function of temperature (K).

The structure of a section is

```
[MAT, 7, 2/  ZA, AWR, LTHR,  0,  0,  0] HEAD                  (LTHR=2)
[MAT, 7, 2/  SB, 0.0,    0,  0, NR, NP/ T_int / W□(T) ] TAB1
[MAT, 7, 0/ 0.0  0.0,    0,  0,  0,  0] SEND
```

7.3.2. Procedures for Incoherent Elastic

This formalism can be used for energies up to 5 eV.

For some moderator materials containing more than one kind of atom, the incoherent elastic cross section is computed as the sum of contributions from two different materials. As an example, H in ZrH_x is given in MAT 0007, and Zr in ZrH_x is given in MAT 0058.

7.4 Incoherent Inelastic Scattering

Inelastic scattering is represented by the thermal neutron scattering law, S(α,β,T), and is defined for a moderating molecule or crystal by

$$\frac{d^2\sigma}{d\Omega dE'}(E \to E', \mu, T) = \sum_{n=0}^{NS} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}}\, e^{-\beta/2}\, S_n(\alpha, \beta, T) \tag{7.6}$$

where (NS+1) types of atoms occur in the molecule or unit cell (*i.e.*, for H_2O, NS=1) and

M_n	Number of atoms of n-type in the molecule or unit cell
T	Moderator temperature (K)
E	Incident neutron energy (eV)
E′	Secondary neutron energy (eV)
B	Energy transfer, β = (E′–E)/kT
α	momentum transfer, α = (E′+E–2μ sqrt(EE′)/A_0kT
A_n	Mass of the n^{th} type atom **A_0** is the mass of the principal scattering atom in the molecule,
σ_{fn}	Free atom scattering cross section of the n^{th} type atom

$$\sigma_{bn} = \sigma_{fn}\left(\frac{A_n + 1}{A_n}\right)^2 \tag{7.7}$$

k	Boltzmann's constant
μ	Cosine of the scattering angle (in the lab system)

The data in File 7 for any particular material contain only the scattering law for the principal scatterer, S(α,β,T), *i.e.*, the 0th atom in the molecule. These data are given as an arbitrary tabulated function. The scattering properties for the ***other atom types*** (n=1,2,...,NS) are represented by ***analytical functions***. Note that the scattering properties of all atoms in the molecule may be represented by analytical functions. In this case there is no principal scattering atom.

In some cases, the scattering properties of other atom types in a molecule or crystal may be described by giving $S_0(\alpha,\beta,T)$ in another material. As an example, H in ZrH_x and Zr in ZrH_x are given in separate MATs.

For high incident energies, α and/or β values may be required that are outside the ranges tabulated for S(α,β). In these cases, the short-collision-time (SCT) approximation should be used as follows:

$$S^{SCT}(\alpha,\beta,T) = \frac{e^{-\left[\frac{(|\alpha|-\beta)^2 T}{4|\alpha|T_{eff}(T)} + \frac{|\beta|}{2}\right]}}{\sqrt{4\pi|\alpha|\frac{T_{eff}(T)}{t}}} \tag{7.8}$$

where $T_{eff}(T)$ is the effective temperature, and the other symbols have their previous meanings.

The constants required for the scattering law data and the analytic representations for the non-principal scattering atoms are given in an array, B(N), N=1,2,...,NI, where NI = 6(NS+1). Six constants are required for each atom type (one 80-character record). The first six elements pertain to the principal scattering atom, n=0.

The elements of the array B(N) are defined as:

B(1) = $M_0 f_0$, the total free atom cross section for the principal scattering atom.

If B(1) = 0.0, there is no principal scattering atom and the scattering properties for this material are completely described by the analytic functions for each atom type in this material.

B(2) = ε, the value of E/kT above which the static model of elastic scattering is adequate (total scattering properties may be obtained from MT=2 as given in File 2 or 3 and File 4 of the appropriate materials).

B(3) = A_0, the ratio of the mass of the atom to that of the neutron that was used to compute α.

$$\left(\alpha = \frac{E' + E - 2\mu\sqrt{EE'}}{A_0} kT\right)$$

B(4) = E_{max}, the upper energy limit for the constant σ_{f0} (upper energy limit in which $S_0(\alpha,\beta,T)$ may be used).

B(5) not used.

B(6) = M_0, the number of principal scattering atoms in the material. (For example, M = 2 for H_2O).

The next six constants specify the analytic functions that describe the scattering properties of the first non-principal scattering atom, (n = 1); *i.e.*, for H_20, this atom would be oxygen if the principal atom were hydrogen.

B(7) = a_1, a test indicating the type of analytic function used for this atom type.
a_1 = 0.0, use the atom in SCT approximation only (see below).
a_1 = 1.0, use a free gas scattering law.
a_1 = 2.0, use a diffusive motion scattering law.

B(8) = $M_1\sigma_{f1}$, the total free atom cross section for this atom type.

B(9) = A_1, effective mass for this atom type.

B(10) = 0.0, B(10) is not used.

B(11) = 0.0, B(11) is not used.

B(12) = M_1, the number of atoms of this type in the molecule or unit cell.

The next six constants, B(13) through B(18), are used to describe the second non-principal scattering atom (n=2), if required. The constants are defined in the same way as for n=1; *e.g.*, B(13) is the same type of constant as B(7).

A mixed S(α,β) method has sometimes been used. Using BeO as an example, the S(α,β) for Be in BeO is combined with that for O in BeO and adjusted to the Be free-atom cross section and mass as a reference. The mixed S(α,β) is used for the principal atom in Eq. (7.6) as if NS were zero. However, ***all*** of the NS+1 atoms are used in the SCT contribution to the cross section.

The scattering law is given by S(α,β,T) for a series of β values. For each β value, the function versus β is given for a series of temperatures. Thus, the looping order is actually first β, then T, then α. S(α,β) is normally a symmetric function of β and only positive values are given. For ortho- and para-hydrogen and deuterium, this is no longer true. Both negative and positive values must be given in increasing value of β and the flag LASYM is set to one.

In certain cases, a more accurate temperature representation may be obtained by replacing the value of the actual temperature, T, that is used in the definition of α and β with a constant, T_0 (T_0 = 0.0253 eV or the equivalent depending of the units of Boltzmann's constant). A flag (LAT) is given for each material to indicate which temperature has been used in generating the S(α,β) data.

For down scattering events with large energy losses and for low temperatures, β can be large and negative. The main contribution to the cross section comes from the region near α + β = 0. Computer precision can become a real problem in these cases. As an example, for water at room temperature, calculations using Eq. (7.6) for incident neutrons at 4 eV require working with products like $e^{80}x10^{-34}$. For liquid hydrogen at 20 Kelvin and for 1 eV transfers, the products can be $e^{300}x10^{-130}$. These very large and small numbers are difficult to handle on most computers, especially 32-bit machines. The LLN flag is provided for such cases: the evaluator simply stores *ln* S instead of S and changes the interpolation scheme accordingly (that is, the normal log-log law changes to log-lin). Values of S = 0.0 like those found in the existing ENDF/B-III thermal files really stand for some very small number less than 10^{-32} and should be changed to some large negative value, such as -999.

7.4.1. Formats for Incoherent Inelastic

The parameters for incoherent inelastic scattering are given in a section of File 7 with MT=4. The following quantities are defined:

LAT	Flag indicating which temperature has been used to compute α and β LAT=0, the actual temperature has been used. LAT=1, the constant T_0 = 0.0253 eV has been used.
LASYM	Flag indicating whether an asymmetric S(α,β) is given LASYM=0, S is symmetric. LASYM=1, S is asymmetric
LLN	Flag indicating the form of S(α,β) stored in the file LLN=0, S is stored directly. LLN=1, ln S is stored.
NS	Number of non-principal scattering atom types. For most moderating materials there will be (NS+1) types of atoms in the molecule (NS≤3).
NI	Total number of items in the B(N) list. NI = 6(NS+1).
B(N)	List of constants. Definitions are given above (Section 7.4).
NR	Number of interpolation ranges for a particular parameter, either β or α .
LT	Temperature dependence flag. The data for the first temperature are given in a TAB1 record, and the data for the LT subsequent temperatures are given in LIST records using the same α grid as for the first temperature.
LI	Interpolation law to be used between this and the previous temperature. Values of LI are the same as those specified for INT in a standard TAB1 interpolation table.
NT	Total number of temperatures given. Note that NT = LT+1.
$\mathbf{T_{eff0}}$	Table of effective temperatures (K) for the short-collision-time approximation given as a function of moderator temperature T(K) for the principal atom.
$\mathbf{T_{eff1}}$, $\mathbf{T_{eff2}}$, $\mathbf{T_{eff3}}$	Table for effective temperatures for the first, second, and third non-principal atom. Given if a_1 = 0.0 only.
NB	Total number of β values given.
NP	Number of α values given for each value of β for the first temperature described, NP is the number of pairs, α and S(α,β), given.
β_{int}, α_{int}	Interpolation schemes used.

The structure of a section is

```
[MAT, 7, 4 /  ZA, AWR,    0, LAT, LASYM,  0] HEAD
[MAT, 7, 4 / 0.0, 0.0, LLN,   0,    NI, NS/ B(N) ] LIST
[MAT, 7, 4 / 0.0, 0.0,   0,   0,    NR, NB/ β_int ] TAB2
[MAT, 7, 4 /  T_0,   β_1,  LT,   0,    NR, NP/ α_int / S(α,β_1,T_0) ] TAB1
[MAT, 7, 4 /  T_1,   β_1,  LI,   0,    NP,  0/ S(α,β_1,T_1) ] LIST
              ------------------------------
              <continue with LIST records for  T_2,T_3,...T_LT+1>
              ------------------------------
[MAT, 7, 4 /  T_0,   β_2,  LT,   0,    NR,  NP/ α_int / S(α,β_2,T_0) ] TAB1
              ------------------------------
          <continue with TAB1 and LIST records for remaining values of β and T>
              ------------------------------
[MAT, 7, 4 / 0.0, 0.0,   0,   0,    NR,  NT/ T_int / T_eff0(T) ] TAB1
              ------------------------------
          <continue with TAB1 records for T_eff1, T_eff2 and/ or T_eff3 if the
            corresponding value of a_1, a_2, or a_3 in B(7), B(13), or B(19) is zero>
              ------------------------------
[MAT, 7, 0 / 0.0, 0.0,   0,   0,     0,   0] SEND
```

If the scattering law data are completely specified by analytic functions (no principal scattering atom type, as indicated by B(1)=0), tabulated values of S(α,β) are omitted and the TAB2 and TAB1 records are not given.

7.4.2. Procedures for Incoherent Inelastic

The data in MF=7, MT=4 should be sufficient to describe incoherent inelastic scattering for incident neutron energies up to 5 eV. The tabulated S(α,β) function should be useful to energies as high as possible in order to minimize the discontinuities that occur when changing to the short-collision-time approximation. The β mesh for S(α,β) should be selected in such a manner as to accurately represent the scattering properties of the material with a minimum of β points. The α mesh at which S(α,β) is given should be the same for each β value of and for each temperature.

Experience has shown that temperature interpolation of S(α,β) is unreliable. It is recommended that cross sections be computed for the given moderator temperatures only. Data for other temperatures should be obtained by interpolation between the ***cross sections***.

REFERENCES

1. Y.D. Naliboff and J.V. Koppel, *HEXSCAT:Coherent Scattering of Neutrons by Hexagonal Lattices*, General Atomic report **GA-6026** (1964).