Update on ENDF-6 Mixed Elastic Scattering Format

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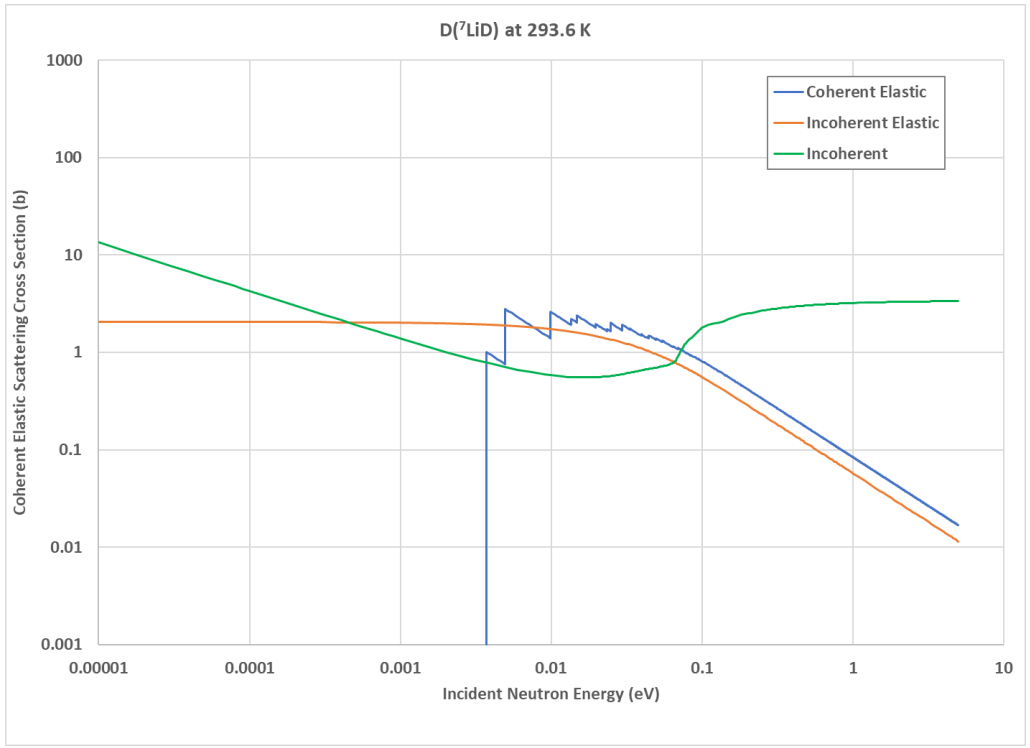
Motivation

- Selected nuclides exhibit both coherent and incoherent elastic scattering effects in the thermal energy range
- A more rigorous thermal elastic scattering treatment is needed to support advanced moderator development
  - Without this treatment Bragg peaks are either neglected (incoherent approximation) or excessive (coherent approximation)
- Mixed Elastic Scattering format is a simple extension to ENDF-6 format
  - Provides support for new capability in GNDS
- No impact on existing TSL evaluations
- Implementation
  - ^{7}LiD and ^{7}LiH TSL evaluations
  - FLASSH TSL evaluation code (to be released)
  - NDEX & FUDGE nuclear data processing codes
  - MC21 & COG neutron transport codes

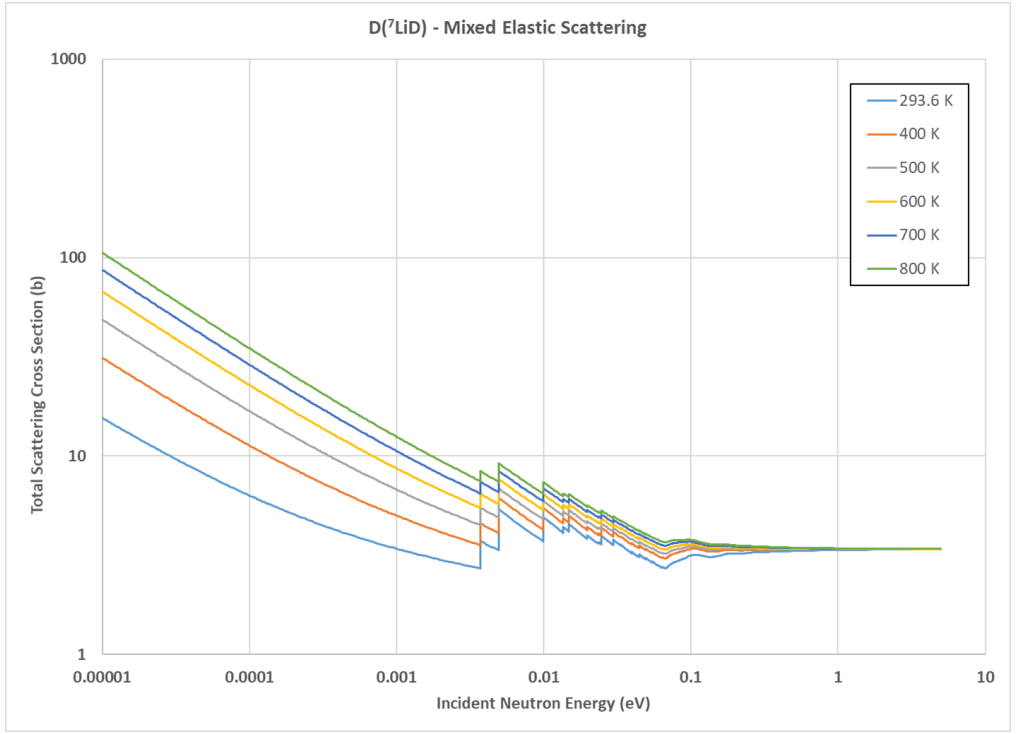
Bound Scattering Cross Sections for Selected Nuclides (b)

Nuclide	σ_c	σ_i	σ_s
^{nat}H	1.7568(10)	80.26(6)	82.02(6)
^{1}H	1.7583(10)	80.27(6)	82.03(6)
^{2}H	**5.592(7)**	**2.05(3)**	**7.64(3)**
^{nat}Li	0.454(10)	0.92(3)	1.37(3)
^{6}Li	0.51(5)	0.46(5)	0.97(7)
^{7}Li	**0.619(11)**	**0.78(3)**	**1.40(3)**
^{nat}B	0.354(5)	1.70(12)	5.24(11)
^{10}B	0.144(8)	3.0(4)	3.1(4)
^{11}B	**5.56(7)**	**0.21(7)**	**5.77(10)**
^{14}N	**11.03(5)**	**0.5(1)**	**11.53(11)**
^{23}Na	**1.66(2)**	**1.62(3)**	**3.28(4)**

D(^{7}LiD) Mixed Elastic Scattering TSL Evaluation

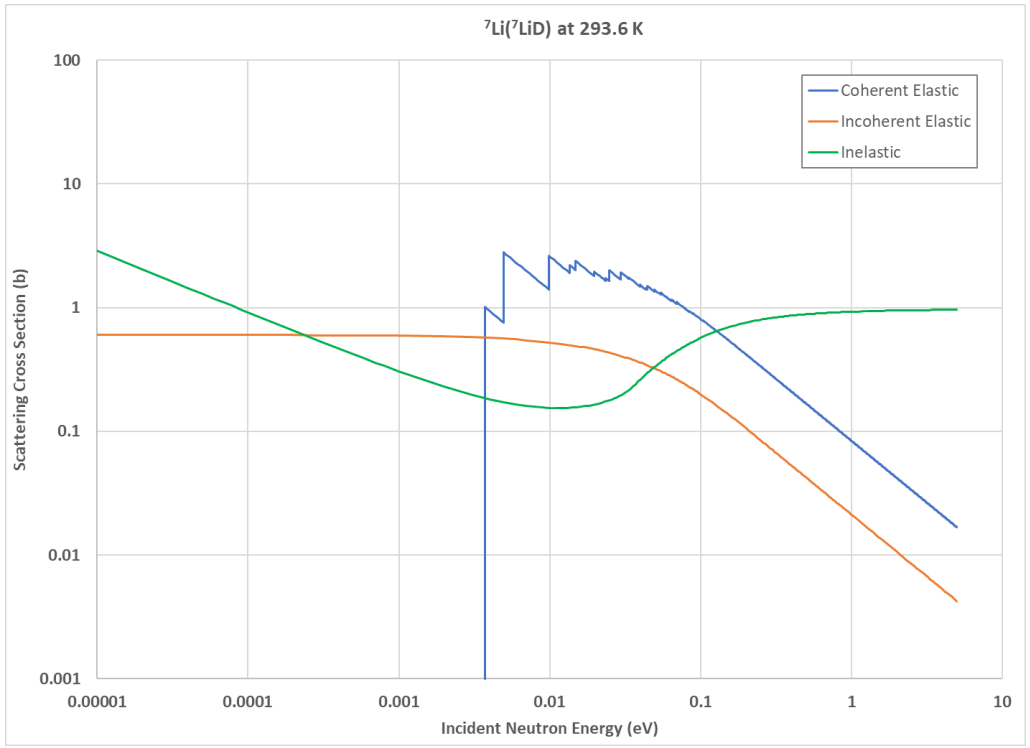


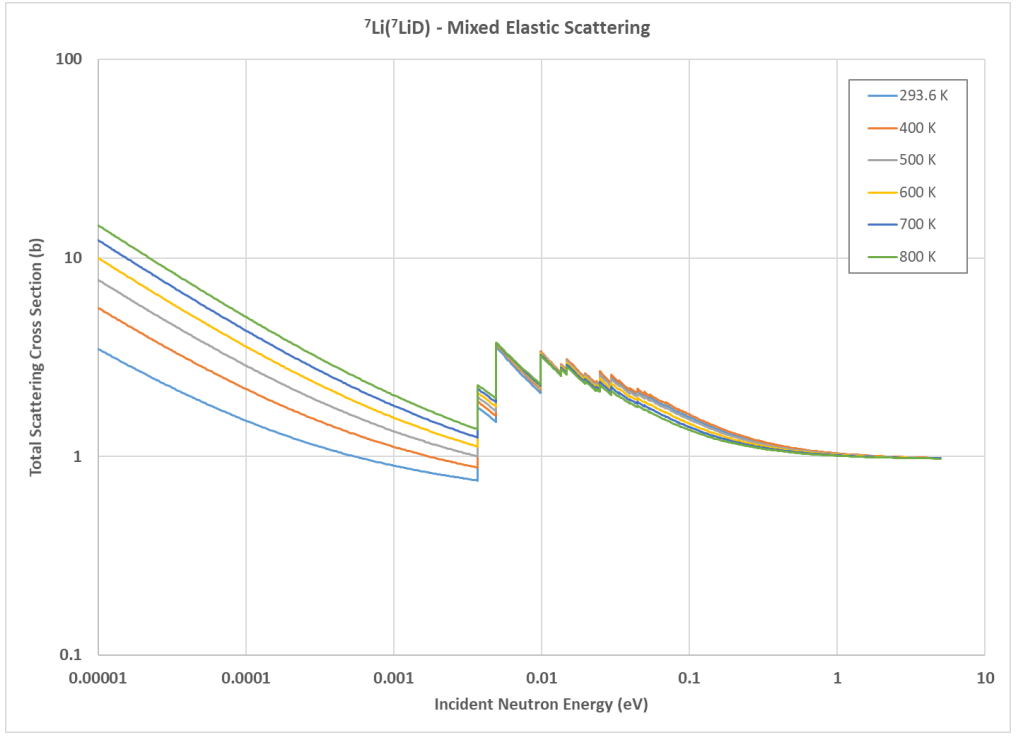
D(^{7}LiD) coherent and incoherent elastic scattering cross sections approximately the same magnitude



Both coherent and incoherent elastic scattering effects captured in NDEX total elastic scattering cross sections

^{7}Li(^{7}LiD) Mixed Elastic Scattering TSL Evaluation





^{7}Li(^{7}LiD) coherent elastic scattering component larger than incoherent elastic scattering component

Bragg scattering more prominent in ^{7}Li(^{7}LiD) total scattering cross sections from NDEX

ENDF-6 Format Proposal

7.4 Mixed Elastic Scattering

Some crystalline materials have mixed coherent and incoherent elastic scattering. The coherent elastic scattering component is represented as described in Section 7.2 and incoherent elastic scattering component is represented as described in Section 7.3.

7.4.1 Formats for Mixed Elastic Scattering

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

ZA, AWR Standard charge and mass parameters.

LTHR Flag indicating which type of thermal data is being represented. LTHR=3 for mixed coherent and incoherent elastic scattering.

T_i Temperature (K).

LT Flag for temperature dependence. The data for the first temperature are given in a TAB1 record. The data for subsequent LT 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, $\mathbf{E}_{int}$ Standard TAB1 interpolation parameters. Use INT=1 (histogram).

NP Number of Bragg edges given.

SB characteristic bound cross section (barns)

NT Number of temperatures.

$W'(T)$ 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=3
[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,T1) ] LIST
  --------------------------
  <repeat LIST for T2, T3, ...TLT>
  --------------------------
[MAT, 7, 2/  SB, 0.0,    0, 0, NR, NT/ Tint / W'(T) ]TAB1
[MAT, 7, 0/0.0, 0.0,    0, 0,  0,  0] SEND
```

7.4.2 Procedures for Mixed Elastic Scattering

The coherent component to the 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.

The incoherent component to the elastic scattering cross section can be used for energies up to 5 eV. The coherent and incoherent components are then added to construct the elastic scattering cross section.

D(^{7}LiD) Mixed Elastic Scattering Example

LTHR=3

```
1.150000+2 1.996800+0          3          0          0          0  15 7  2
2.936000+2 0.000000+0          5          0          1       3374  15 7  2
      3374          1                                              15 7  2
1.235573-3 2.67690-34 2.471146-3 5.24780-34 3.706719-3 3.757353-3  15 7  2
4.942291-3 1.386287-2 6.177864-3 1.386287-2 7.413437-3 1.386287-2  15 7  2
9.884583-3 2.595574-2 1.112016-2 2.595574-2 1.235573-2 2.595574-2  15 7  2
1.359130-2 2.992438-2 1.482687-2 3.549502-2 1.606245-2 3.549502-2  15 7  2
⋮
4.399400-2 4.399400-2 4.399400-2 4.399400-2 4.399400-2 4.399400-2  15 7  2
4.399400-2 4.399400-2                                             15 7  2
2.054202+0 0.000000+0          0          0          1          6  15 7  2
         6          2                                              15 7  2
2.936000+2 8.937898+0 4.000000+2 1.047985+1 5.000000+2 1.213545+1  15 7  2
6.000000+2 1.390890+1 7.000000+2 1.575652+1 8.000000+2 1.765328+1  15 7  2
0.000000+0 0.000000+0          0          0          0          0  15 7  0
1.150000+2 1.996800+0          0          1          0          0  15 7  4
0.000000+0 0.000000+0          0          0          6          0  15 7  4
3.395004+0 1.976285+2 1.996800+0 5.000000+0 0.000000+0 1.000000+0  15 7  4
0.000000+0 0.000000+0          0          0          1        300  15 7  4
       300          4                                              15 7  4
2.936000+2 0.000000+0          5          0          1        200  15 7  4
       200          4                                              15 7  4
2.059042-2 4.931327-4 2.163677-2 5.181545-4 2.273629-2 5.444438-4  15 7  4
2.389168-2 5.720646-4 2.510579-2 6.010840-4 2.638160-2 6.315727-4  15 7  4
⋮
```

Coherent Elastic

Bound incoherent scattering cross section

Incoherent Elastic

Inelastic

Status

- ENDF-6 format proposal available in endf6man GitLab repository at NNDC
  - Sample evaluations available for H(^{7}LiH), ^{7}Li(^{7}LiH), D(^{7}LiD), ^{7}Li(^{7}LiD)
  - Sample NDEX processed data in .xlsx format
- Conditionally approved during Nov 2020 CSEWG Meeting
  - Pending implementation in AMPX or NJOY
- Evaluation code implementation
  - FLASSH – complete
  - NJOY – ?
- Processing Code Implementation
  - NDEX – complete
  - FUDGE – complete
  - AMPX – ?
  - NJOY – in progress