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Format requirements of thermal neutron scattering data in an nuclear data format to succeed the ENDF format

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Format requirements of thermal neutron scattering data in a nuclear data format to succeed the ENDF format

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INTRODUCTION

In November 2012, the Working Party on Evaluation Cooperation Subgroup 38 (WPEC-SG38) began with the task of developing a nuclear data format and supporting infrastructure to replace the now nearly 50 year old ENDF format. The first step in this process is to develop requirements for the new format and infrastructure. In this talk, I will review the status of ENDF's Thermal Scattering Law (TSL) formats as well as support for this data in the GND format (from which the new format is expected to evolve). Finally, I hope to begin a dialog with members of the thermal neutron scattering community so that their data needs can be accurately and easily accommodated by the new format and tools, as captured by the requirements document.

During this discussion, we must keep in mind that the new tools and format must:

- Support what is in existing data files;
- Support new things we want to put in data files;
- Be flexible enough for us to adapt it to future unanticipated challenges.

ENDF HISTORY

For context we review the current state of ENDF thermal neutron scattering formats and libraries and understand how these evolved into their current forms.

Evolution of ENDF's TSL formats

The Thermal Scattering Law (TSL) data describe the situation where neutrons scatter off a material with a low enough energy that its de Broglie wavelength cannot resolve individual nuclei. TSL covers neutron coherent elastic, incoherent elastic and (coherent and incoherent) inelastic scattering events. Thermal neutron scattering is typically formulated using the theory of Van Hove [1].

TSL data for incoherent inelastic scattering date from very first ENDF format specifications in 1966 [2]. Coherent and incoherent elastic scattering were originally stored as Legendre moments in the MF=4 files. Incoherent inelastic cross sections are computed as

$$\frac{d^2\sigma}{dE'd\Omega}(E,T) = \sum_{n=0}^{NS} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} \mathcal{S}_n(\alpha,\beta,T) \quad (1)$$

Here

$$\alpha = \frac{E' + E - 2\mu\sqrt{E'E}}{AkT} \quad \text{and} \quad \beta = \frac{E' - E}{kT} \quad (2)$$

To tabulate data for this parameterization, one must store *S(α,β,T)* interpolation tables and the free cross sections σ_{bn} in ENDF's MF=7 format.

In the early 1990's, parameterized coherent and incoherent elastic scattering were added to ENDF format [3]. Coherent elastic scattering is given by

$$\frac{d^2\sigma}{dE'd\Omega}(E,T) = \frac{1}{2\pi E} \sum_{i=1}^{E_i<E} s_i(T)\delta(\mu-\mu_i)\delta(E-E') \quad (4)$$

where

$$\mu_i = 1 - \frac{2E_i}{E} \quad (5)$$

Here, we must store the structure factor *s(E,T)* tables in ENDF's MF=7 (note these factors are given as a histogram in ENDF, hence the notation in Eq. (4)). Incoherent elastic scattering is given by

$$\frac{d^2\sigma}{dE'd\Omega}(E,T) = \frac{\sigma_b}{4\pi} e^{-2EW'(T)(1-\mu)} \delta(E-E') \quad (6)$$

Here must store the characteristic bound cross section σ_b and the Debye-Waller integral *W(T)* tables in ENDF's MF=7 files.

No provision has ever been made for covariance on thermal scattering data.

Evolution of the contents of the ENDF library

Major changes to the ENDF library have happened sporadically since the 1970's. Fig. 1 illustrates the history of new and modified evaluations in the ENDF library from Refs [4-7].

Original evaluations were performed by General Atomics using GASKET, HEXCAT, GAKER and ZREND codes [4]. These evaluations were included in the ENDF/B-III release of the ENDF library. Later evaluations were almost exclusively done by R.E. MacFarlane using LEAPR module of NJOY [8].

LEAPR is an evolution of UK's LEAP code [8]. The LEAPR module computes the TSL data from the phonon spectrum of the material in question. The derivation of the formulas are theoretically interesting and involves several approximations. Then end result of the calculation is

$$\mathcal{S}(\alpha,\beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt\, e^{i\beta t} e^{-\gamma(t)} \quad (7)$$

with

$$\gamma(t) = \alpha \int_{-\infty}^{\infty} d\omega \rho(\omega) \left(1 - e^{-i\omega t}\right) \frac{e^{-\omega/2}}{2\omega \sinh(\omega/2)} \tag{8}$$

The target material's phonon spectrum is *ρ(ω)* and this is the primary input to LEAPR.

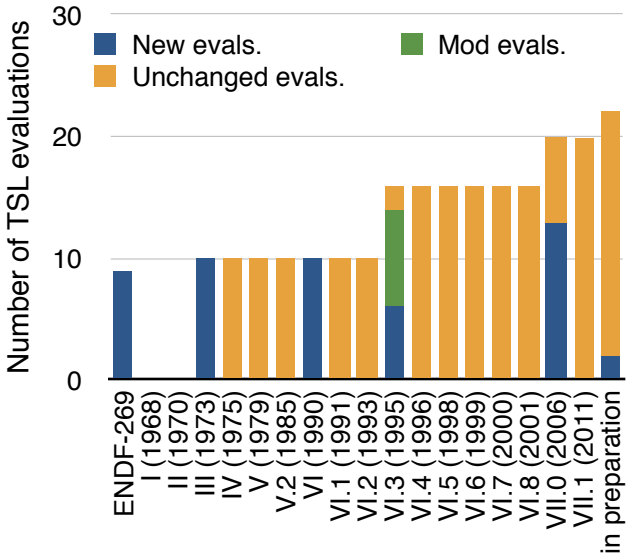

Fig. 1. Number of new and modified thermal neutron scattering evaluations in each ENDF/B library release. Also shown are the evaluations listed in Ref [1].

FORMAT AND TOOLS TO SUCCEED ENDF

In November 2012, WPEC Subgroup 38 (SG38) "Beyond the ENDF format: A modern nuclear database structure", was formed. More information is available at https://www.oecd-nea.org/science/wpec/sg38/**.** At this and subsequent meetings, an initial set of foundational requirements for the top level data hierarchy were established:

- The hierarchy should reflect our understanding of nuclear reactions and decays, and clearly and uniquely specify all data.
- It should support storing multiple representations of the same quantity simultaneously (e.g. evaluated and processed data).
- Should support both inclusive and exclusive reaction data (i.e., discrete reaction channels as well as sums over those channels).
- It should eliminate redundancy where possible.
- It should make use of general-purpose data containers also developed in this project.

The preliminary implementation of a replacement ENDF format is LLNL's Generalized Nuclear Data (GND) format [9]. GND contains a sample TSL implementation by C. Mattoon. This implementation mirrors the ENDF format in structure and function, but with XML markup.

We are now at a stage where we are drafting detailed requirements for the format. We need to address following issues:

- What should we store? Cross sections, parameter tables, or raw phonon spectra?
- Where in the hierarchy will TSL data reside?
- How will we store covariance on tabulated data?
- How will TSL evaluations be connected to higher energy evaluations where we can resolve individual nuclei?

Also, there is a more fundamental question: is the LEAPR formalism the best choice for a representation of the reactions involved or should some of the approximations be relaxed?

Development of a top-level hierarchy requirements document is in progress and we would like you to help contribute. The discussions that I have with you in this meeting will be integrated into the requirements document. Also, if you would like to aid in the drafting of the document, please see me. The deadline for the requirements document is May 2014's WPEC meetings.

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