FLASSH 1.0: Thermal Scattering Law Evaluation and Cross Section Generation

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Abstract. The Full Law Analysis Scattering System Hub (*FLASSH*) is an advanced code which evaluates the thermal scattering law (i.e. TSL, S(α,β)) for thermal scattering cross sections and resonance Doppler broadening. The ability to accurately capture these two key cross section features is dependent on accurate, high fidelity TSL evaluations. *FLASSH* 1.0 provides advanced physics capabilities resulting in an improved, generalized TSL to most accurately represent the lattice dynamics within any material. This improved TSL will allow for consistent analysis in both the thermal and epithermal energy ranges. The features for TSL analysis are packaged within the *FLASSH* GUI for easy user interface along with data output in many file formats including ENDF File 7 and ACE files.

1 Introduction

The Full Law Analysis Scattering System Hub (*FLASSH*) code was developed to provide high-fidelity thermal scattering data to support applications in advanced reactor modelling, criticality safety, and neutron science. *FLASSH* is an advanced code which calculates the thermal scattering law (i.e. TSL, S(α,β)) for both thermal scattering cross section and resonance Doppler broadening. These features in the cross section are both fundamentally driven by target atom vibrations, which are impacted b the nature of the chemical binding and temperature of the lattice. To accurately capture the structure's impact on cross section, the material property of the TSL must be evaluated to include an accurate representation of the physical phenomena which correlate the atoms. The advanced physics in *FLASSH* 1.0 introduces generalized formulations to most accurately represent the lattice dynamics for any material.

2 Evaluation inputs

The features of the TSL are packaged within the *FLASSH* GUI for easy user interface. The GUI allows user to visually step through the evaluation process with the added benefit of built-in error checks and automatic input file formatting. The *FLASSH* GUI also provides automatic default values to inform user inputs as well as tool tips which describe variables and special formatting.

In generating the inputs for TSL evaluation, *FLASSH* begins in the GUI with a main Configuration window. An example of this window with the automatically loaded default values is shown in Figure 1. The only required inputs for standard, solid materials would be the mass, free atom cross section, and a labelling number for the evaluation. With the basic framework in place, the GUI will proceed to any other required information. For all evaluations, the material density of states (DOS) must be provided by the user. Depending on the type of evaluation, additional input of the material crystal structure may be requested, but for all materials which have been evaluated up through ENDF/B-VIII.0, these inputs are available within the GUI itself.

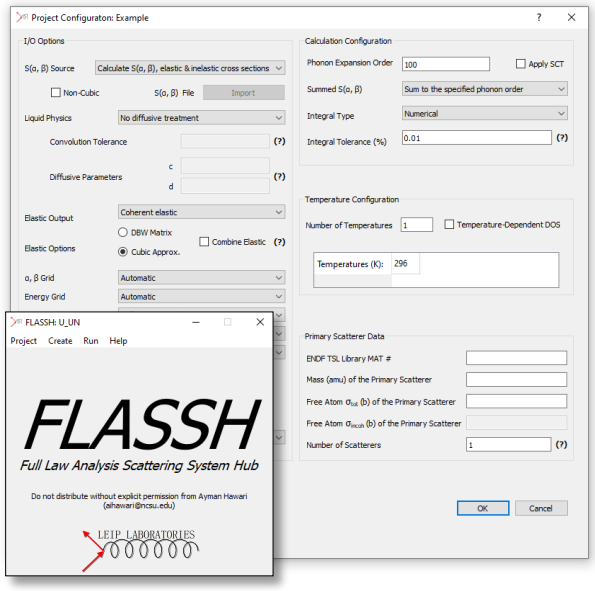

Fig. 1. *FLASSH* GUI main configuration window with default pre-loaded values.

While a simple, solid evaluation only requires the input of the mass, free atom cross section, DOS, and a

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selection of material reference number, *FLASSH* offers customization options to the advanced evaluator. Some of these options include automatic α and β gridding for liquids or hydrides. The outgoing energy grid can also be manually specified which is necessary for oscillatory materials such as hydrides. Users may also specify the maximum energy of the evaluation. The default value is set to 5.0 eV; however, for some materials, a higher or lower energy many be required to asymptote to the appropriate free atom cross section.

As a part of the GUI, users may choose the format of the output data. These include the standard ENDF-6 formatted file, ACE files, and user output of the data. Plots of the evaluated data are also generated by the GUI to allow the evaluator to assess the quality of the TSL and associated cross sections.

3 *FLASSH* TSL evaluations

The TSL is a material property which defines the interference and non-interference effects within a material [1]. In a thermal reactor system, as the neutron slows to energies on the order 1 eV or less, the de Broglie wavelength of the neutron will be on the same order of magnitude as the interatomic spacing of the material lattice [1-2]. At this point, the neutron interacts not only with the individual atoms but also with the lattice structure. The available structure effects which contribute to the interactions are quantified in the TSL.

3.1 TSL formulations

In its most basic form, the TSL is defined in two parts: the self scattering law (S_s) and the distinct scattering law (S_d) such that the total TSL $S(\alpha,\beta)$ is equal to

$$S(\alpha,\beta) = S_s(\alpha,\beta) + S_d(\alpha,\beta). \quad (1)$$

Traditional approximations then assume that the atoms are bound with harmonic forces which allow the TSL to be written in terms of a series expansion, called the phonon expansion. Additional approximations which assume a cubic structure or equivalent, symmetrical forces as well as identical atoms within the unit cell were commonly applied. The incoherent approximation which assumes that the distinct contributions are negligible would be applied such that using historical codes, the TSL would be evaluated such that

$$S(\alpha,\beta) = \sum_{p\geq 1} S_s^p(\alpha,\beta). \quad (2)$$

FLASSH is able to reproduce this historical, approximated version of the TSL, but in order to accurately capture the physics of the materials, *FLASSH* also offers a generalized formation of the TSL which includes the first summation term of the distinct contributions as well as a generalized non-cubic formulation. This "1-phonon" approximation introduces the exchange modes which were historically neglected and generalizes the structure to allow the material's directionality to define the TSL.

The TSL is directly proportional to the double differential scattering cross section:

$$\frac{\partial^2\sigma}{\partial\mu\partial E'} = \frac{1}{2k_BT}\sqrt{\frac{E'}{E}}[\sigma_{inc}S_s(\alpha,\beta) + \sigma_{coh}S(\alpha,\beta)]. \quad (3)$$

As such, the improved formulations of the TSL directly improve the cross sections produced from *FLASSH*. A comparison of the key features in *FLASSH* against similar TSL evaluation codes is shown in Figure 2.

	NJOY/LEAPR	NJOY+NCrystal	*FLASSH*
Coherent Elastic Supported Materials	Graphite, Beryllium, Beryllium Oxide, Aluminum, Lead, Iron	Any material, any structure	Any material, any structure
Coherent Inelastic	**No**	**Yes!**	**Yes!**
Optional Scattering Lengths Input (real and imaginary)	**No**	**No**	**Yes!**
Integral Against Alpha Differential Cross Section	Numerical		Default: Numerical Optional: Analytical
α, β Gridding	User Input		Default: Automatic grid Optional: User input
Parallel Computing	**No**	**No**	**Yes!**
Graphical User Interface	**No**	**No**	**Yes!**
Syntax and Error Checking	**No**	**No**	**Yes!**
Create Inputs for Compatible Codes	**No**	**No**	**Yes!**
Remove Cubic Approximation	**No**	**No**	**Yes!**
Remove Atom Site Approximation	**No**	**No**	**Yes!**
Remove Incoherent Approximation	**No**	**No**	**Yes!**
Remove Short Collision Time (SCT) Approximation	**No**	**No**	**Yes!** (Optional SCT)
Liquid Physics Options	Free Gas & Schofield Models		Free Gas, Schofield, & Langevin Models

Fig. 2. Comparison of *FLASSH* features with commonly used codes such as the LEAPR module of NJOY and NCrystal [3-4].

3.2 Elastic scattering applications

In evaluating the elastic scattering, *FLASSH* includes the option of producing both coherent and incoherent elastic cross sections. *FLASSH* supports both the current ENDF-6 formatting for elastic as well as the updated formatting to include mixed elastic materials as shown in Figure 3. In evaluating the coherent elastic, both cubic and non-cubic (Debye Waller matrix) formulations are implemented [5]. Both the cubic and non-cubic coherent elastic formulations are generalized to allow for any materials structure. It is vital that for generalized, non-cubic formulations that a non-cubic formational of the cross section be used across all portions of the total cross section (e.g. inelastic non-cubic as well).

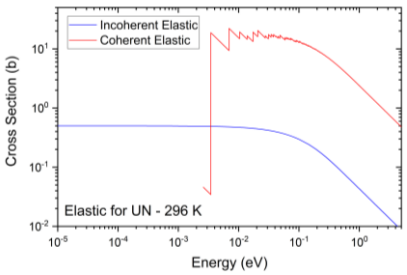

Fig. 3. Coherent and incoherent elastic cross section (mixed elastic) evaluated for uranium nitride.

3.3 Inelastic scattering applications

The inelastic scattering portion of the cross section is evaluated in light of the material nature. While solids typically contain coherent elastic, liquids must be treated to include the appropriate diffusive components. Within *FLASSH*, the Schofield, Langevin, and free gas models are available [6]. For these models, the diffusive dimensionless parameters of *c* relaxation time and *d* diffusivity are input.

For the solid portion of the inelastic cross section, again both cubic and non-cubic generalized formulations are available [7]. The directional nature of the non-cubic formation requires input of the directional DOS rather than an average DOS as used for the cubic evaluation. The resulting cross section impacts can be seen in Figure 4.

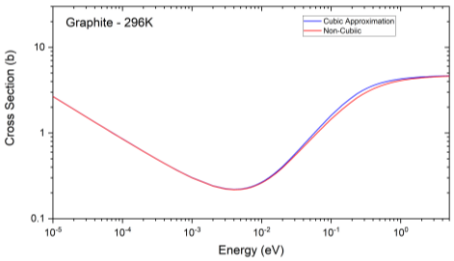

Fig. 4. Inelastic cross section evaluated for graphite at 296 K.

3.4 Advanced physics

While the atom site and cubic approximations have been relaxed in the coherent and incoherent cross sections, to remove the remaining incoherent approximation required additional physics to capture the distinct effects of the TSL. Using the 1-phonon approximation, the first phonon order of the distinct contribution was formulated and included in *FLASSH* [8].

The 1-phonon distinct contributions are by nature non-cubic, and having the foundation of the generalized non-cubic elastic and inelastic cross sections allows for the direct application of the 1-phonon terms to the total TSL. The 1-phonon module requires the additional input of the polarization vectors and associated frequencies for a material. These inputs can be generated using codes such as phonopy [9]. With the 1-phonon contribution, the TSL now accurately represents the material structure factors allowing for direct comparison with experimental data as shown in Figure 5.

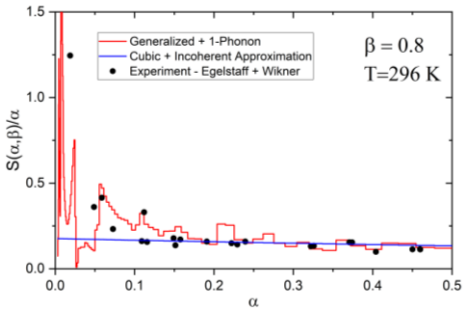

Fig. 5. TSL of graphite evaluated using *FLASSH* and compared to experimental data [10-11].

4 Application of the TSL to cross sections

4.1 Thermal scattering cross sections

The TSL as evaluated using *FLASSH* provides a high-fidelity description of the material interaction characteristics. Using this generalized TSL with 1-phonon contributions, the calculated data can be directly compared to experiment for benchmarking at the TSL level. However, the integral application of the TSL to the scattering cross section allows a second point of comparison. For strongly directional materials such as graphite, the inclusion of the generalized formulation with 1-phonon contributions is vital to accurately predicting the cross section.

As clearly seen in Figure 5, the TSL improvements with the advanced physics TSL from *FLASSH* are observed in the structure seen in the TSL and the experimental data. The integration of this TSL into the cross section, as shown in Figure 6, demonstrates the impact of these TSL changes on the thermal cross section.

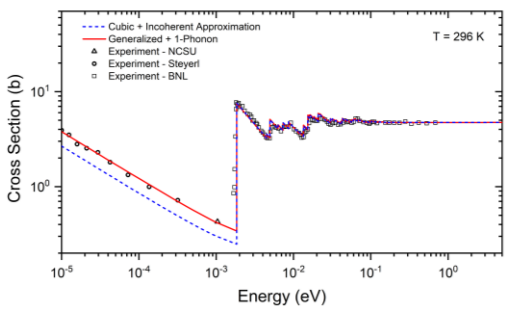

Fig. 6. Total cross section of graphite evaluated using *FLASSH* and compared to experimental data [12-14].

4.2 Doppler broadening

The application of the TSL is not limited to the thermal scattering cross sections. As a material property which quantifies chemical binding effects, the TSL can be applied to describe the structure impacts on the atoms' velocity distributions. This structure informed distribution incorporates the interaction material into the evaluation of the temperature processes of Doppler broadening.

Traditionally, Doppler broadening would assume the atoms of the system followed a free gas or Maxwellian velocity distribution. As such, they were considered to be unbound. However, a more complete description of the atomic motion includes the binding effects. Using the TSL to describe the velocity distribution in Doppler broadening most accurately captures the crystalline solid effects.

An approximation which improves the free gas broadening uses the DOS (e.g. material structure information) to derive an effective temperature. *FLASSH* automatically uses this effective temperature to broaden any absorption resonances, taking advantage of the material details already included for the TSL evaluation. *FLASSH* also includes a crystalline solid (TSL) broadening. An example of the *FLASSH* broadening is given in Figure 7.

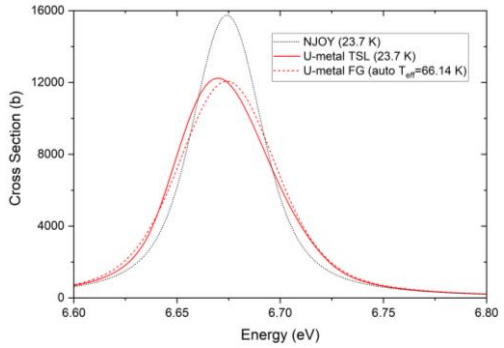

Fig. 7. Absorption cross section of uranium metal evaluated using *FLASSH* and compared to NJOY [3].

Using the high-fidelity TSL from *FLASSH* which includes the advanced physics options, both the thermal scattering and Doppler broadened cross sections are consistently evaluated with the details of the material structure defining the interactions.

5 Conclusions

FLASSH 1.0 is an advanced code which provides high-fidelity TSL evaluations which can be applied to both thermal scattering cross sections as well as resonance Doppler broadening. The advanced physics implemented within *FLASSH* allows for direct benchmarking of the TSL as well as the resulting cross sections. These advanced features in *FLASSH* are easily accessible within the code's GUI.

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