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Full Law Analysis Scattering System Hub (FLASSH)

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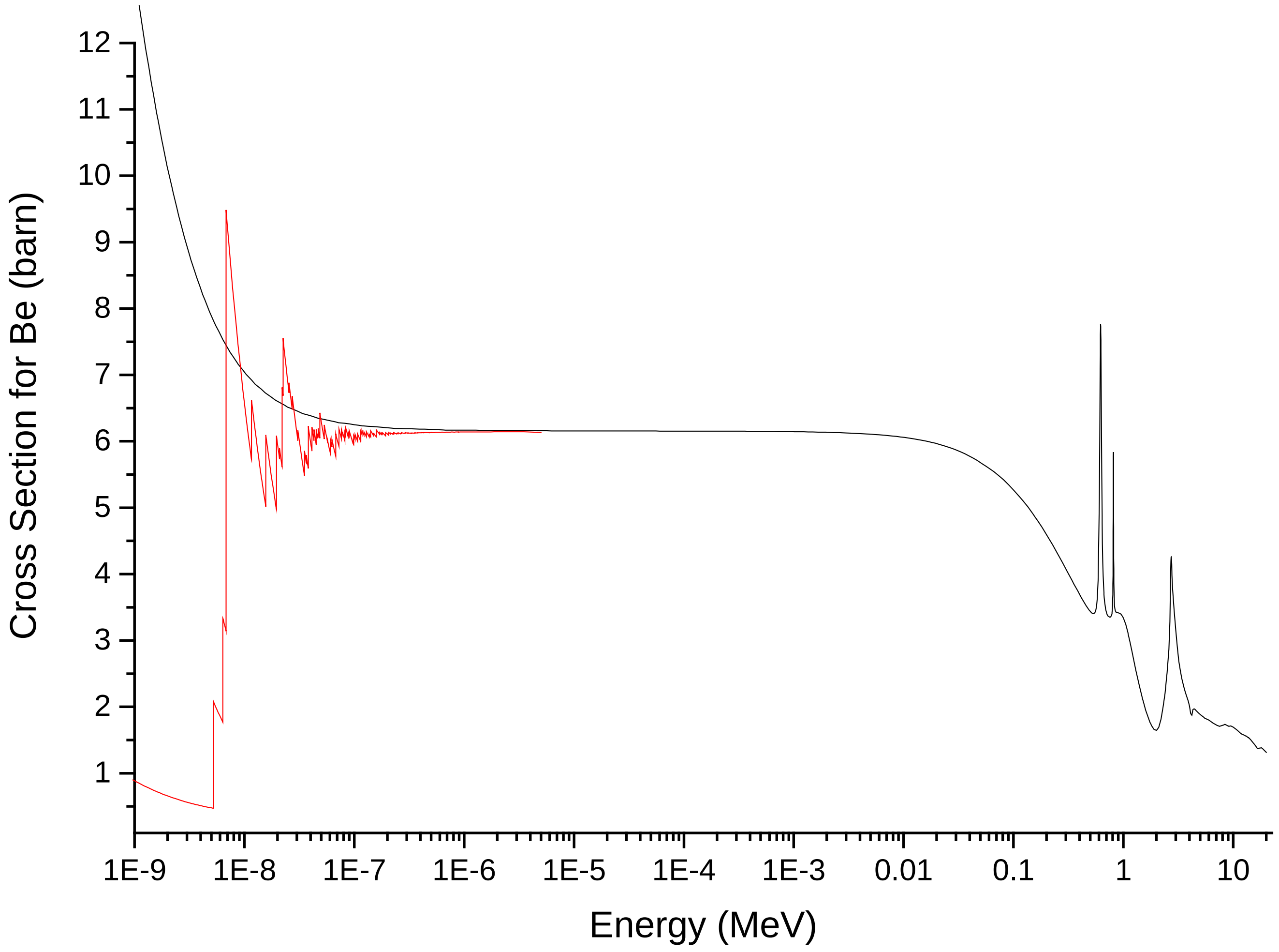
Outline

- Overview of thermal neutron scattering theory
- Overview of FLASSH Code Development
- Inelastic Scattering under Incoherent Approximation
- Coherent Inelastic Scattering with One-phonon Correction
- Coherent Elastic Scattering with Debye-Waller matrix
- Summary

Thermal Neutron Scattering in Matter



Thermal Neutron Scattering in Matter

- Thermal neutrons are characterized by energies and de Broglie wave length that are on the order of excitation energy and separation distance in the medium in which they interact

- The scattering behavior of thermal neutrons are quantified by the double differential cross section using the scattering law $S(\alpha, \beta)$

$$\frac{d^2\sigma}{d\mu dE'} = \frac{\sigma_b}{2k_B T}\sqrt{\frac{E'}{E}}S(\alpha,\beta)$$

- The scattering law $S(\alpha, \beta)$, also known as the dynamic structure factor, describes the energy states of motions and the structure constitution of the interaction medium

Thermal Neutron Scattering in Matter

- $S(\alpha,\beta)$ is made up of self and distinct terms and can be written as

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

- The neutron scattering cross section can be further written as

$$\frac{d^2\sigma}{d\mu dE'} = \frac{1}{2k_B T}\sqrt{\frac{E'}{E}}\left(\sigma_{coh} S(\boldsymbol{\kappa},\omega) + \sigma_{inc} S_s(\boldsymbol{\kappa},\omega)\right)$$

- Harmonic approximation: interatomic forces are proportional to displacement from equilibrium position. Scattering law can be expanded

$$S_d = \sum_{i=0} {}^{i}S_d \qquad\qquad S_s = \sum_{i=0} {}^{i}S_s$$

Phonon Expansion of the Scattering Law

- Coherent elastic scattering

$$\left(\frac{d^2\sigma}{d\mu dE'}\right)_{coh} = \frac{\sigma_{coh}}{2k_BT}\sqrt{\frac{E'}{E}}\left[{}^0S_d + {}^0S_s\right]$$

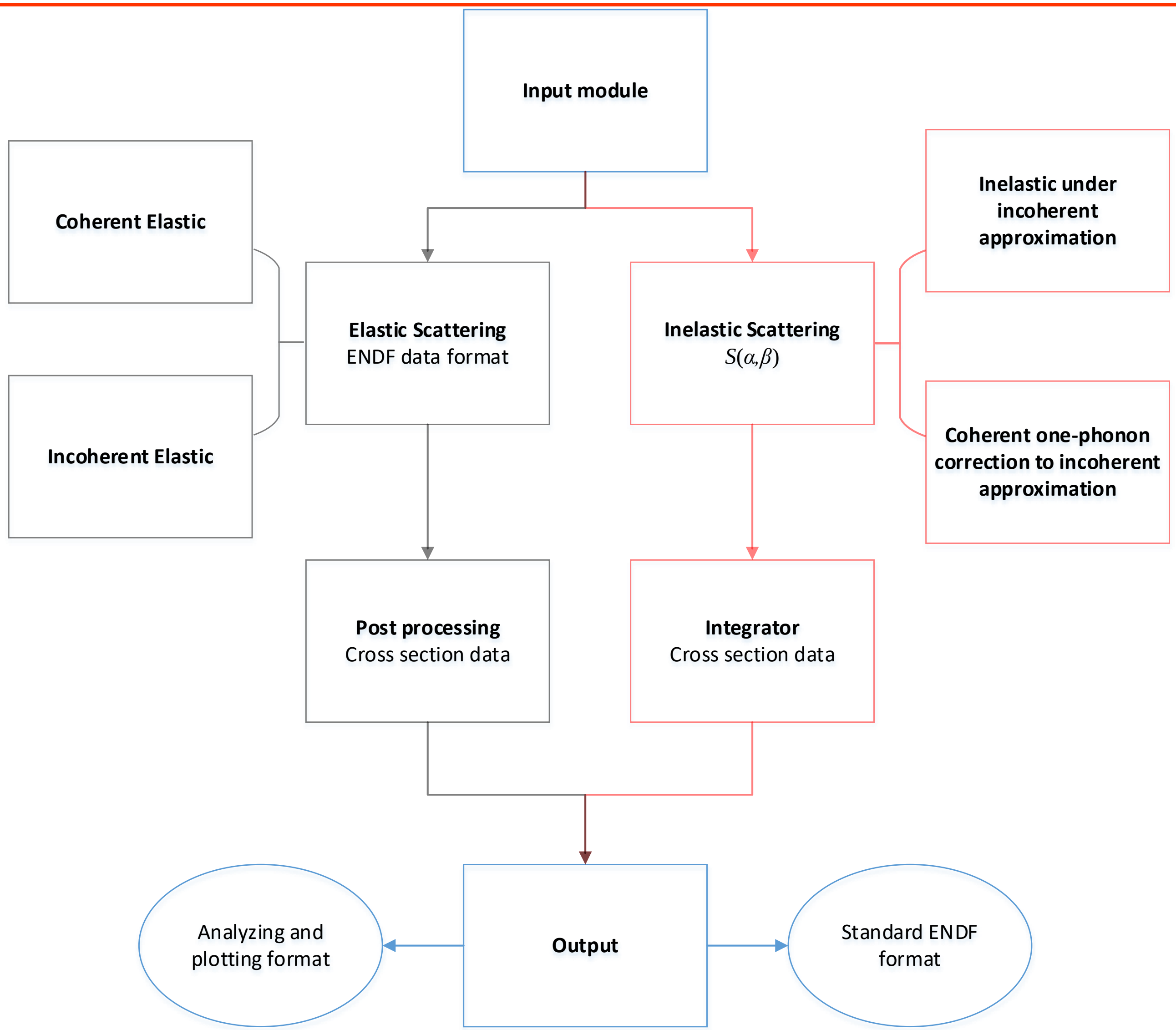
- Incoherent elastic scattering

$$\left(\frac{d^2\sigma}{d\mu dE'}\right)_{inc} = \frac{\sigma_{inc}}{2k_BT}\sqrt{\frac{E'}{E}}\left[{}^0S_s\right]$$

- Inelastic scattering under incoherent approximation

$$\left(\frac{d^2\sigma}{d\mu dE'}\right)_{inela} = \frac{\sigma_{coh}+\sigma_{inc}}{2k_BT}\sqrt{\frac{E'}{E}}\left[{}^1S_s + {}^2S_s \ldots\right]$$

FLASSH Code Flow

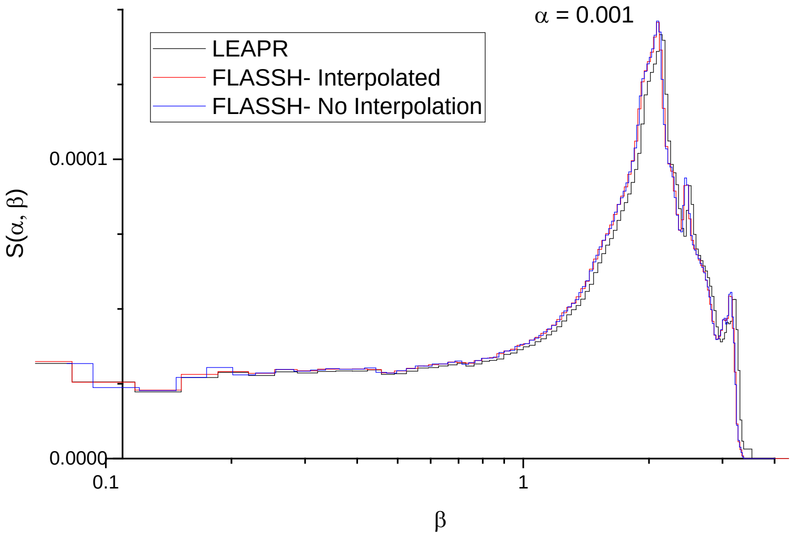


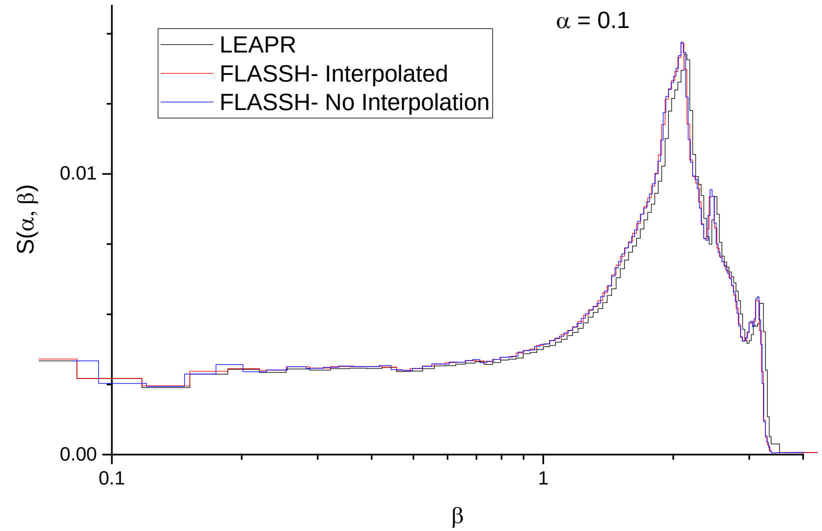
FLASSH Code Features

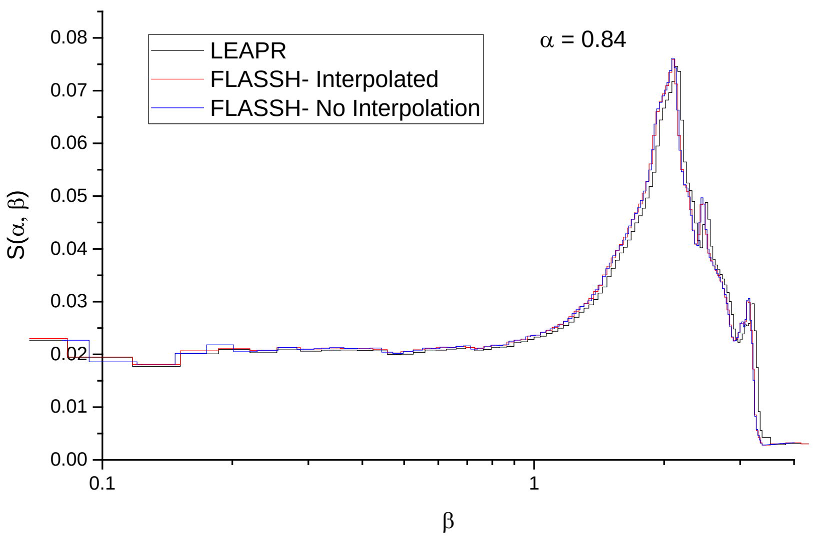
	LEAPR+THERMR	FLASSH
Coherent inelastic	N/A	Implemented
Coherent elastic	Approximate	Exact
Short Scattering Time (SCT) approximation	Yes	No
Integral against α differential cross section	Numerical	**Default: Analytical** Optional: Numerical
α, β gridding	User input	**Default: Automatic grid** Optional: User input
Parallel Computing	N/A	**Yes** Using OpenMP
Graphic User Interface	N/A	Yes

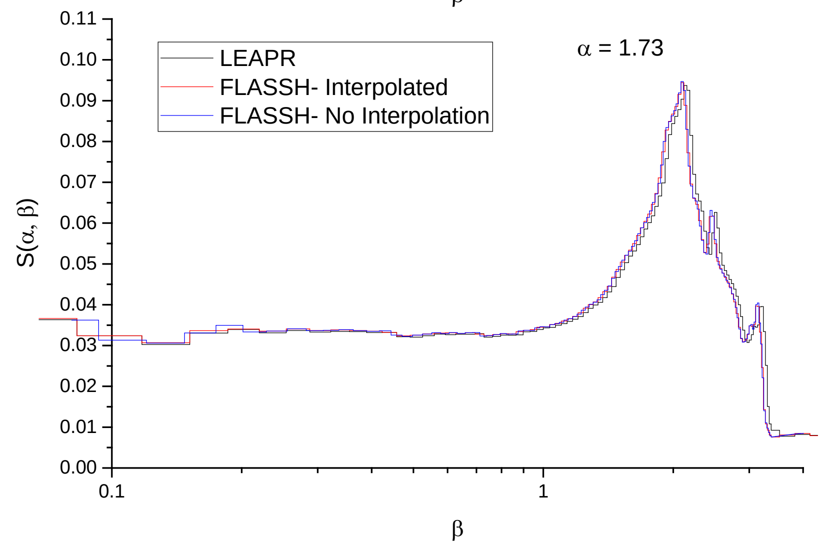
FLASSH Example

Scattering Law $S(\alpha, \beta)$

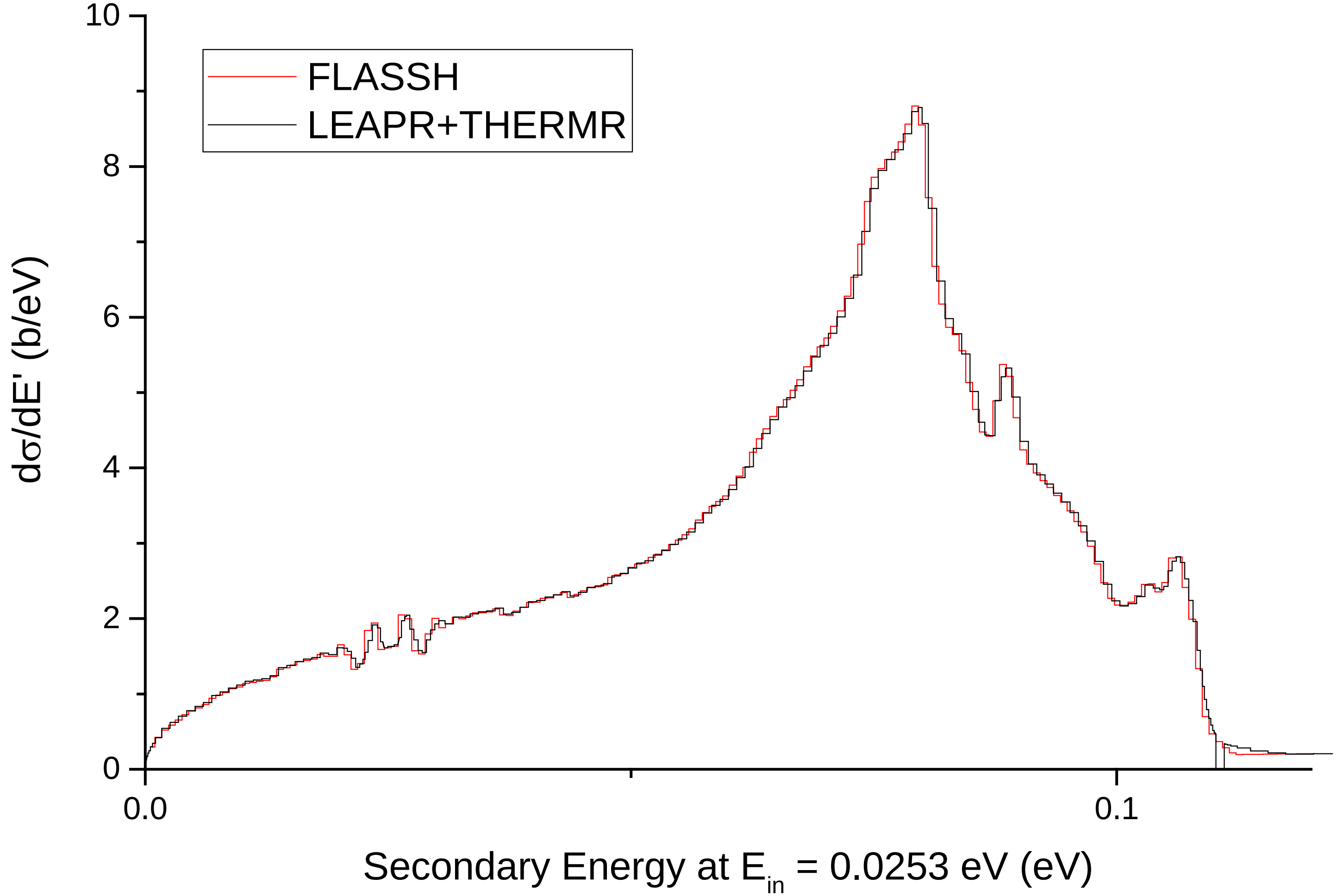




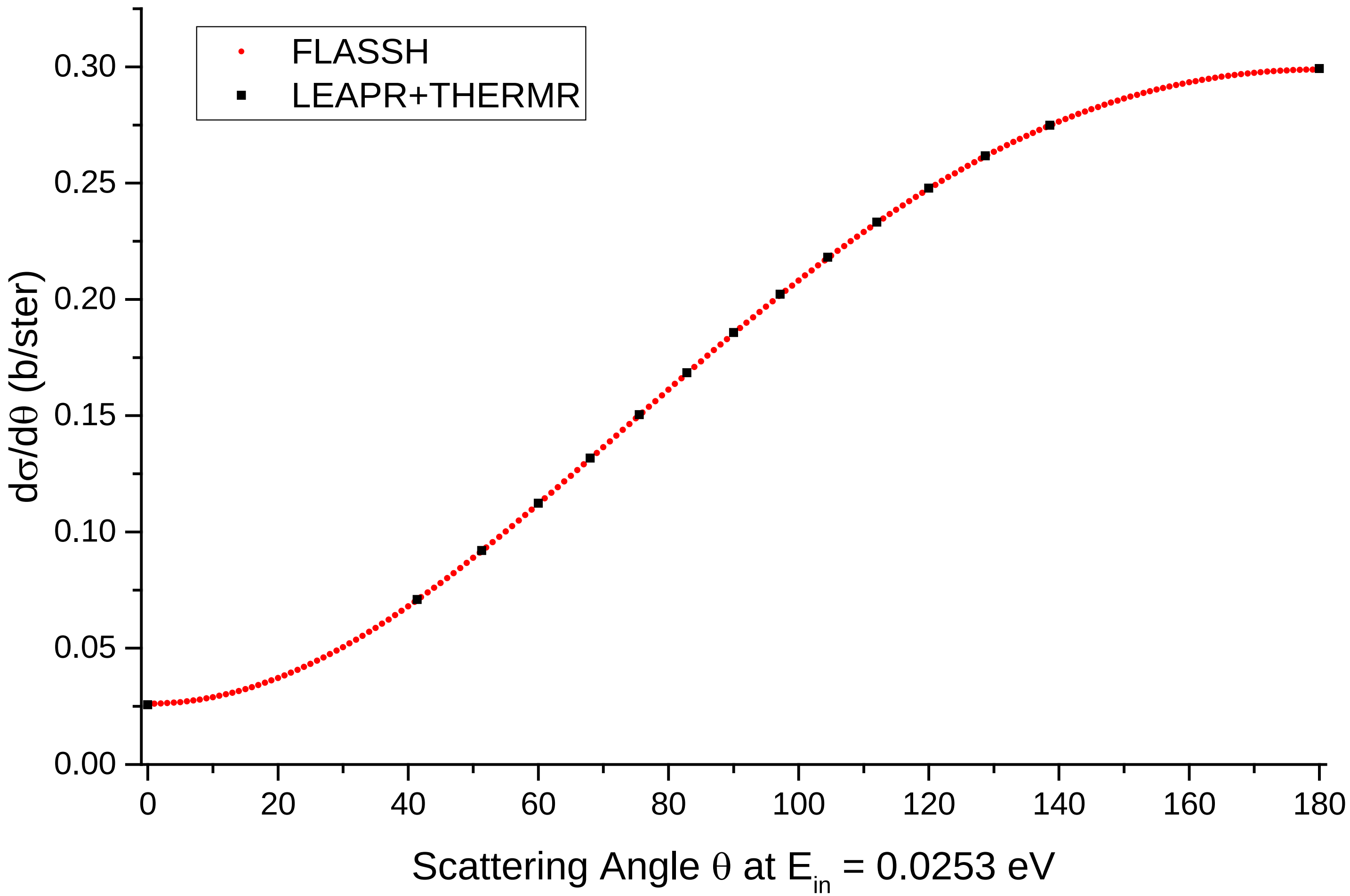




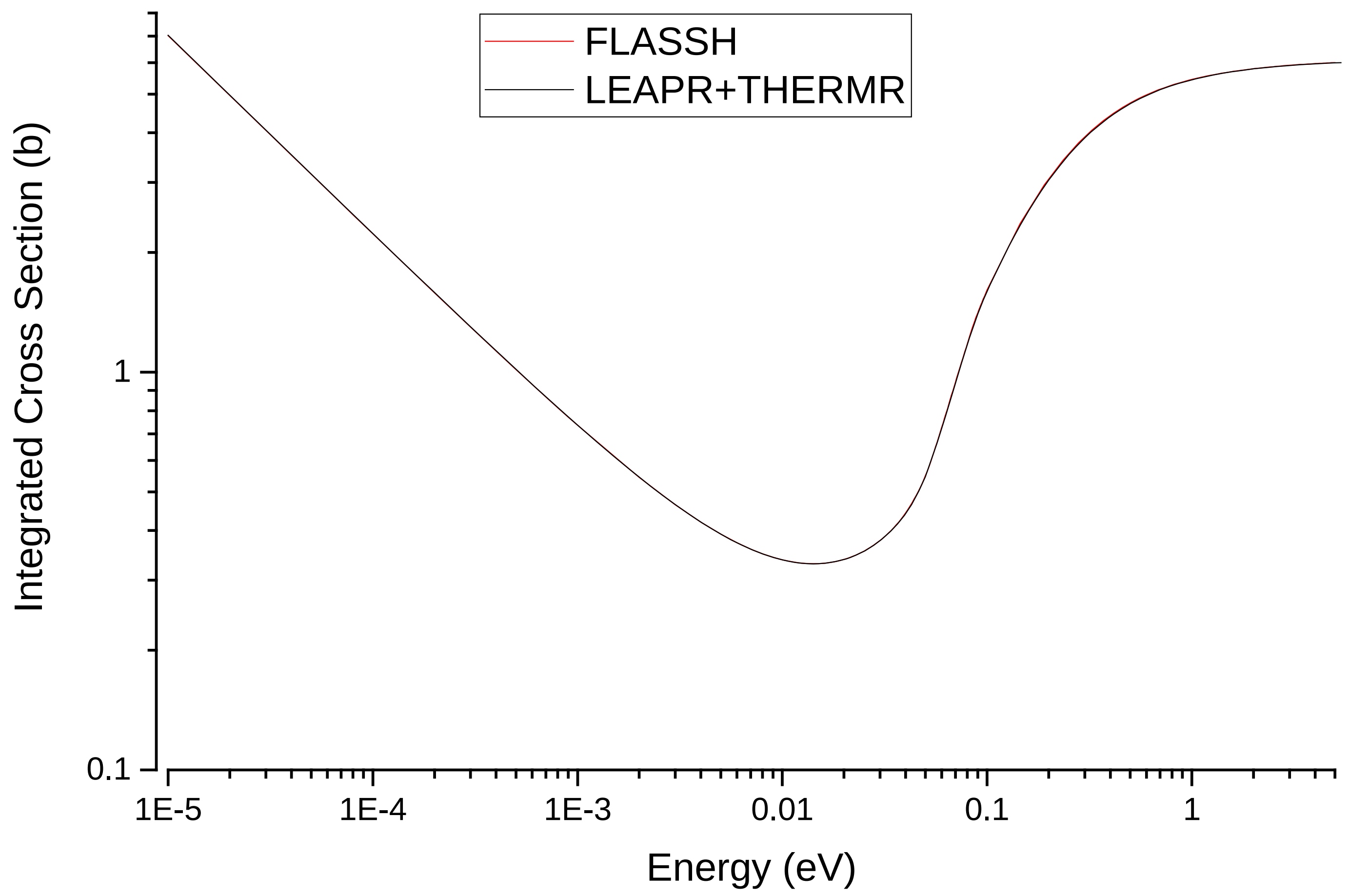
Differential Scattering Cross Section



Differential Scattering Cross Section



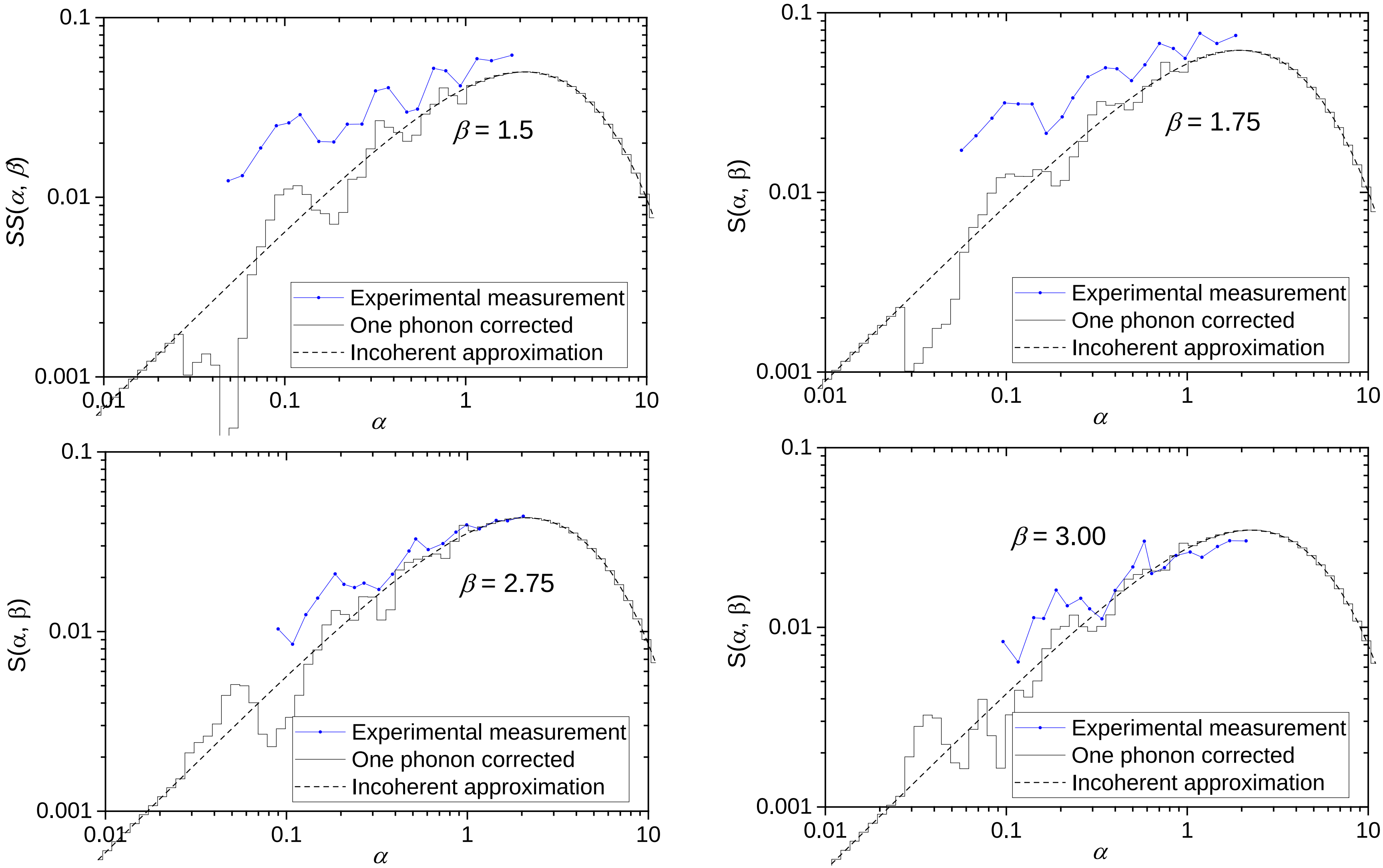
Integrated Cross Section



Coherent inelastic one-phonon correction routine

	FLASSH
Supported structure	Any crystal structure
Supported material	Any material
Compound material	Yes
Debye-Waller Factor	Exact
Polarization vector	Exact
Sampling of the full reciprocal space	Yes
Structure Factor	Exact

One-phonon Corrected Scattering Law $S(\alpha,\beta)$



Coherent Elastic Routine

	LEAPR	FLASSH
Supported structure	Hexagonal, FCC, BCC	Any crystal structure
Supported material	Graphite, beryllium, beryllium oxide, aluminum, lead, iron	Any material
Compound material	2 elements with ratio 1:1	Any number of elements with any ratio
Cubic Approximation	Yes	No
Atom sites approximation	Yes	No
Coherent Elastic Scattering Cross Section	Over Ewald Sphere	On every reciprocal lattice point
Need to modify source code if calculating other materials	Yes	No

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Approximations of the LEAPR Coherent Elastic Routine

$$B_{il}(\mu) = \frac{\hbar}{2M_\mu}\int_0^{\omega_m} \frac{\rho_{il,\mu}(\omega)}{\omega}\coth\left(\frac{\hbar\omega}{2k_B T}\right)d\omega$$

$$\lambda = \int_0^\infty \frac{1}{\beta}\rho_{tot}(\beta)\coth\left(\frac{\beta}{2}\right)d\beta$$

$$W_\mu(\boldsymbol{\kappa}) = \frac{1}{2}\boldsymbol{\kappa}\cdot\mathbf{B}(\mu)\cdot\boldsymbol{\kappa}$$

Cubic Approx. →

$$W = \frac{\lambda}{Ak_B T}$$

$$F(\boldsymbol{\kappa}) = \sum_\mu \overline{b}_\mu e^{i\boldsymbol{\kappa}\cdot\mathbf{d}} e^{-W_\mu}$$

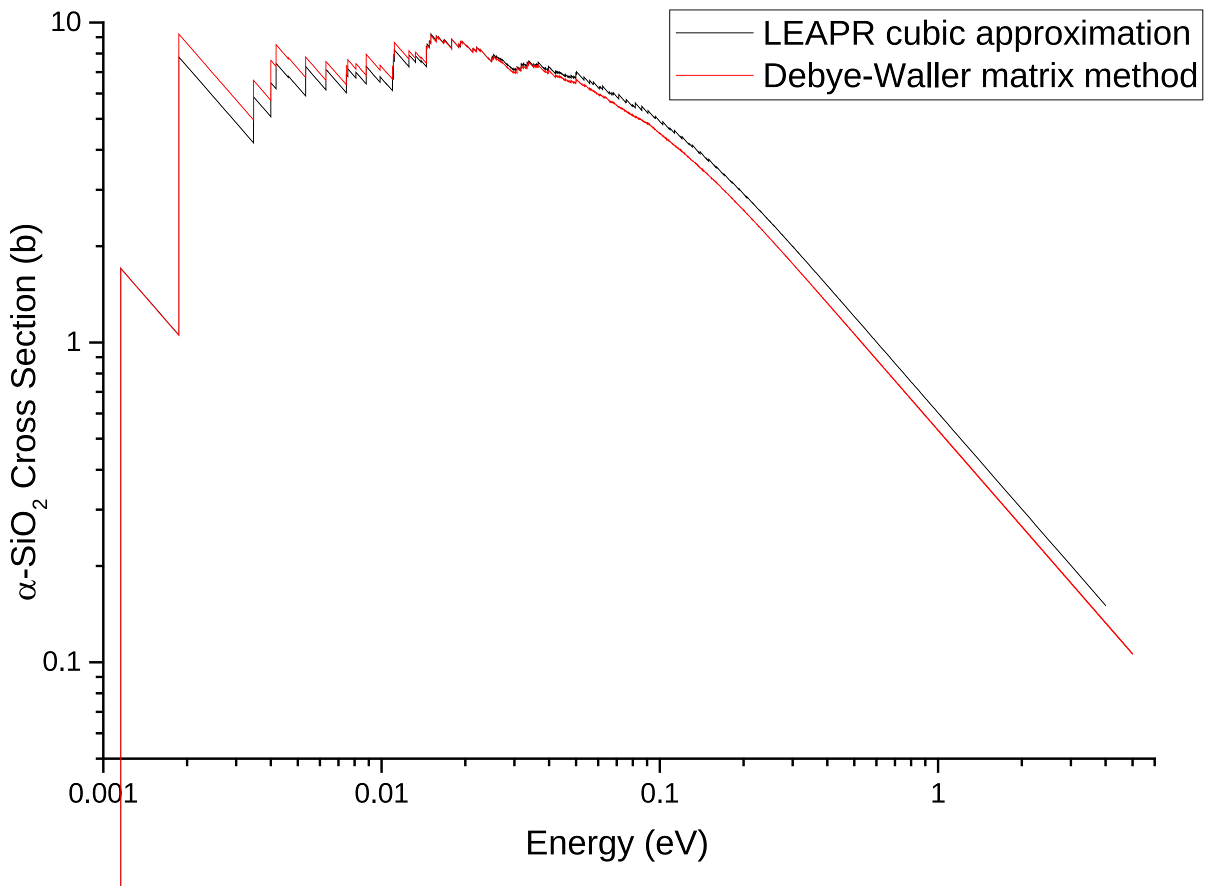
Atom Site Approx. →

$$F(\boldsymbol{\kappa}) = e^{-W}\sum_j \overline{b}\cdot e^{i\boldsymbol{\kappa}\cdot\mathbf{d}_j}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh\ el} = N\frac{(2\pi)^3}{v_0}\sum_{\boldsymbol{\tau}}\delta(\boldsymbol{\kappa}-\boldsymbol{\tau})\left|F(\boldsymbol{\kappa})\right|^2$$

$$\sigma_{coh}(E,\mu) = \frac{1}{E}\sum_{E_i<E}\frac{f_i}{\tau_i}e^{-4WE_i}\delta(\mu-\mu_i)$$

Coherent Elastic Cross Section of α-SiO_2



- The calculation shows around 15% divergence at low and high energies between the two methods in the cross sections of α-SiO_2.

Code Implementation

- Calculations and ENDF TSL library formatting modules were implemented by FORTRAN 95 using modulus design
- MF=1, MT=451 formatting was done by Python
- Parallel computing was realized by OpenMP 4.0 bindings
- GUI implemented by cross platform QT® C++ API

Summary

- The more general coherent elastic and coherent inelastic calculation routines were implemented.
- Approximations such as SCT approximation, cubic approximation, atom site approximation and incoherent approximation were removed or relaxed in FLASSH.
- Compared FLASSH results to NJOY results and experimental measurements.
- FLASSH is designed using modern C++ and FORTRAN95 language with GUI and parallel computation capability.

Acknowledgements

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