Status of TSL Code Development at NCSU

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Outline

- Overview of Code Development
- Inelastic Scattering under Incoherent Approximation
- Coherent Inelastic Scattering with One-phonon Correction
- Coherent Elastic Scattering with Debye-Waller matrix
- Summary
**Code Flow**

- **Input module**
  - Elastic Scattering
    - ENDF data format
  - Inelastic Scattering
    - $S(\alpha,\beta)$

- **Post processing**
  - Cross section data

- **Integrator**
  - Cross section data

- **Output**
  - Analyzing and plotting format
  - Standard ENDF format

- **Coherent Elastic**
  - Incoherent Elastic
  - Coherent one-phonon correction to incoherent approximation
  - Inelastic under incoherent approximation
# Code Features

<table>
<thead>
<tr>
<th>Feature</th>
<th>LEAPR+THERMR</th>
<th>New Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coherent inelastic</td>
<td>N/A</td>
<td>Implemented</td>
</tr>
<tr>
<td>Coherent elastic</td>
<td>Approximate</td>
<td>Exact</td>
</tr>
<tr>
<td>Short Scattering Time (SCT) approximation</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Integral against $\alpha$ differential cross section</td>
<td>Numerical</td>
<td>Default: Analytical  Optional: Numerical</td>
</tr>
<tr>
<td>$\alpha$, $\beta$ gridding</td>
<td>User input</td>
<td>Default: Automatic grid  Optional: User input</td>
</tr>
<tr>
<td>Parallel Computing</td>
<td>N/A</td>
<td>Yes Using OpenMP</td>
</tr>
<tr>
<td>Graphic User Interface</td>
<td>N/A</td>
<td>Yes</td>
</tr>
</tbody>
</table>
Evaluation Example
Evaluation Example
Evaluation Example
Scattering Law $S(\alpha, \beta)$

- $\alpha = 0.001$
- $\alpha = 0.1$
- $\alpha = 0.84$
- $\alpha = 1.73$
Differential Scattering Cross Section

Secondary Energy at $E_{in} = 0.0253$ eV (eV)

Scattering Angle $\theta$ at $E_{in} = 0.0253$ eV

New Code LEAPR+THERMR

New Code LEAPR + THERMR
Integrated Cross Section

Integrated Cross Section (b)

New Code
LEAPR + THERMR

Energy (eV)
Coherent inelastic one-phonon correction routine

<table>
<thead>
<tr>
<th>Feature</th>
<th>New Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>Supported structure</td>
<td>Any crystal structure</td>
</tr>
<tr>
<td>Supported material</td>
<td>Any material</td>
</tr>
<tr>
<td>Compound material</td>
<td>Yes</td>
</tr>
<tr>
<td>Debye-Waller Factor</td>
<td>Exact</td>
</tr>
<tr>
<td>Polarization vector</td>
<td>Exact</td>
</tr>
<tr>
<td>Sampling of the full reciprocal space</td>
<td>Yes</td>
</tr>
<tr>
<td>Structure Factor</td>
<td>Exact</td>
</tr>
</tbody>
</table>
One-phonon Corrected Scattering Law $S(\alpha, \beta)$

![Graphs showing scattering law with different values of $\beta$.]
## Coherent Elastic Routine

<table>
<thead>
<tr>
<th></th>
<th>LEAPR</th>
<th>New routine</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Supported structure</strong></td>
<td>Hexagonal, FCC, BCC</td>
<td>Any crystal structure</td>
</tr>
<tr>
<td><strong>Supported material</strong></td>
<td>Graphite, beryllium, beryllium oxide, aluminum, lead, iron</td>
<td>Any material</td>
</tr>
<tr>
<td><strong>Compound material</strong></td>
<td>2 elements with ratio 1:1</td>
<td>Any number of elements with any ratio</td>
</tr>
<tr>
<td><strong>Cubic Approximation</strong></td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td><strong>Atom sites approximation</strong></td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td><strong>Coherent Elastic Scattering Cross Section</strong></td>
<td>Over Ewald Sphere</td>
<td>On every reciprocal lattice point</td>
</tr>
<tr>
<td><strong>Need to modify source code if calculating other materials</strong></td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>
The calculation shows around 15% divergence at low and high energies between the two methods in the cross sections of $\alpha$-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 the new code.

- Tested the new code by comparing to NJOY result and experimental measurements.

- The new code is designed using modern C++ and FORTRAN95 language with GUI and parallel computation capability.