Towards a better thermal neutron scattering law generation: oClimax + NJOY2016

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Thermal Scattering Overview

• Overall objectives:
  – Use double differential thermal scattering and vibrational spectroscopy measurements to benchmark and improve thermal scattering evaluations.

• Preform measurement at SNS (ORNL):
  – Use ARCS and SEQUOIA for double differential scattering.
  – Use VISION for phonon spectrum measurements.
    • Key collaborators at ORNL: Goran Arbanas, (Mike Dunn).
    • Scientists at SNS: Alexander Kolesnikov, Doug Abernathy, Luke Daemen,

• Advantages:
  – New measurements have much better energy and angle resolution compared to old data.
  – Can measure different type of samples (liquid, solid, mixtures, compounds).
  – Measurements can be done at variety of temperatures starting from 5K
  – Tremendous amount of different experimental information helps constrain and overcome modeling deficiencies.
Thermal Scattering Experimental Needs

- **Time-of-flight SEQUOIA and ARCS**
- **Total Cross Section**
- **Phonon Spectrum**
- **DFT, oClimax**
- **VISION**
- **MCNP with resolution**
- **Benchmark $K_{eff}$**
- **ENDF NJOY TSL**
- **Method. 1**
- **Method. 2**
- **Triple Axis**

Diagram: Connections between different experimental methods and cross-sections.
## Completed Experiments

<table>
<thead>
<tr>
<th>Moderators</th>
<th>SEQUOIA (Ω: 3-58° in 1° increments)</th>
<th>ARCS (Ω: 3-125° in 1° increments)</th>
<th>VISION (at 5 K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light Water (H₂O)</td>
<td>Eᵢ: 55, 160, 250, 600, 1000, 3000, 5000 meV Temp: 300 K</td>
<td></td>
<td>YES</td>
</tr>
<tr>
<td>Polyethylene (CH₂)</td>
<td>Eᵢ: 55, 160, 250, 600, 1000, 3000, 5000 meV Temp: 300 K</td>
<td>Eᵢ: 50, 100, 250, 700 meV Temp: 5, 295 K</td>
<td>YES</td>
</tr>
<tr>
<td>Quartz (SiO2)</td>
<td></td>
<td>Eᵢ: 50, 100, 250, 700 meV Temp: 5, 295, 573, 823, 873 K Thickness: 3.175, 6.35 mm</td>
<td>YES</td>
</tr>
<tr>
<td>Teflon ((C₂F₄)ₙ)</td>
<td>Eᵢ: 50, 100, 250, 700 meV Temp: 5, 300, 500 K</td>
<td></td>
<td>NO</td>
</tr>
<tr>
<td>Lucite (C₅O₂H₈)</td>
<td>Eᵢ: 50, 100, 250, 700 meV Temp: 5, 300, 400 K</td>
<td></td>
<td>YES</td>
</tr>
<tr>
<td>Concrete (mixture)</td>
<td>Eᵢ: 50, 100, 250, 700 meV Temp: 5, 300 K</td>
<td></td>
<td>NO</td>
</tr>
</tbody>
</table>
Thermal scattering – evaluation methodology

START

CASTEP DFT code output: Atomic displacements and frequencies

oCLimax
Calculates $S(Q,\omega)$ from DFT for VISION instrument geometry
Output: $S(Q,\omega)$

VISION experimental $S(Q,\omega)$

VISION $S(Q,\omega)$
Comparable to DFT $S(Q,\omega)$?

NO

Adjust phonon frequencies

YES

Transform $S(Q,\omega)$ to GDOS

VISION $S(Q,\omega)$

NJOY2016 output: ENDF thermal library

$S(\alpha,\beta)$

Comparable to Experimental DDSCS and $\sigma_t$?

NO

S($\alpha,\beta$)

YES

Serious Problem: Improve Theory (and NJOY)

DONE: NEW $S(\alpha,\beta)$

$S(\alpha,\beta)$

RED = Experimental data used
Polyethylene Experimental Data and Evaluation

VISION data used to validate and adjust the evaluation
Experimental data used for validation:
- Double differential scattering
- Total cross section from the literature
Polyethylene Criticality Benchmarks

- The new RPI evaluation and the ENDF/B-VIII.0 give similar results.
- There are some discrepancies between the benchmarks and simulation.
Lucite (C$_5$O$_2$H$_8$)$_n$
Total cross section and benchmarks

- RPI library represents a clear improvement to K-effective.
- ENDF/B-VIII.0 is similar to free gas treatment.
Possible Phonon Expansion Issues?

- Phonon expansion:

\[ e^{\gamma(t)} = e^{-\alpha \lambda} \sum_{n=0}^{\infty} \frac{1}{n!} \left[ P(\beta) e^{i\beta t} e^{-\beta/2} \right]^n \]

\[ S(\alpha, \beta) = e^{-\alpha \lambda} \sum_{n=0}^{\infty} \frac{1}{n!} \frac{1}{\alpha^n} \frac{1}{2\pi} \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} P(\beta') e^{i\beta' t} e^{-\beta'/2} d\beta' \right]^n dt \]
Possible Phonon Expansion Issues?
Possible Phonon Expansion Issues?

- Ice 5 K VISION
- Ice-1h 5 K DFT+oCLimax n=10 scaled
- Ice-1h 5 K DFT+oCLimax n=1 scaled

\(S(Q,\omega)\)

Energy (meV)

\((C_5O_2H_8)_n\)

- DFT+oClimax n=10 scaled
- DFT+oClimax n=1 scaled

Total Cross-Section (b)

Energy (meV)

- Torres 2006 T=115 K
- RPI ice-1h DFT+oClimax
- Ice-1h ENDF/VIII optimized
- Ice-1h ENDF/VIII Original Theoretical Curve

\((C_5O_2H_8)_n\)

- ENDF/B-VIII.0
- RPI DFT+oClimax
- Sibona et. al.
- K. Drozdowicz 1989

Total Cross-Section (b)

Energy (meV)
Questions?
Supplemental Slide

![Graph showing GDOS for (C_2H_4)_n vs Energy (meV)]

- GDOS (Arbitrary units)
- Energy (meV)

- (C_2H_4)_n
- H-(C_2H_4)_n DFT+oClimax adjusted n=1

![Graph showing GDOS for (C_2H_4)_n vs Energy (meV)]

- GDOS (Arbitrary units)
- Energy (meV)

- (C_2H_4)_n
- CASTEP