Update on Thermal Scattering Research at RPI

Report to NDAG

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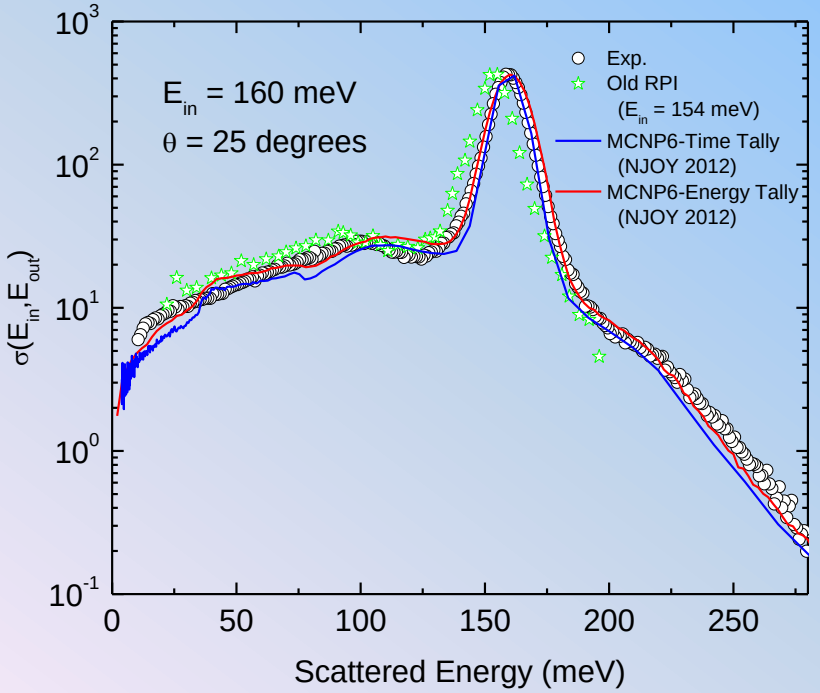
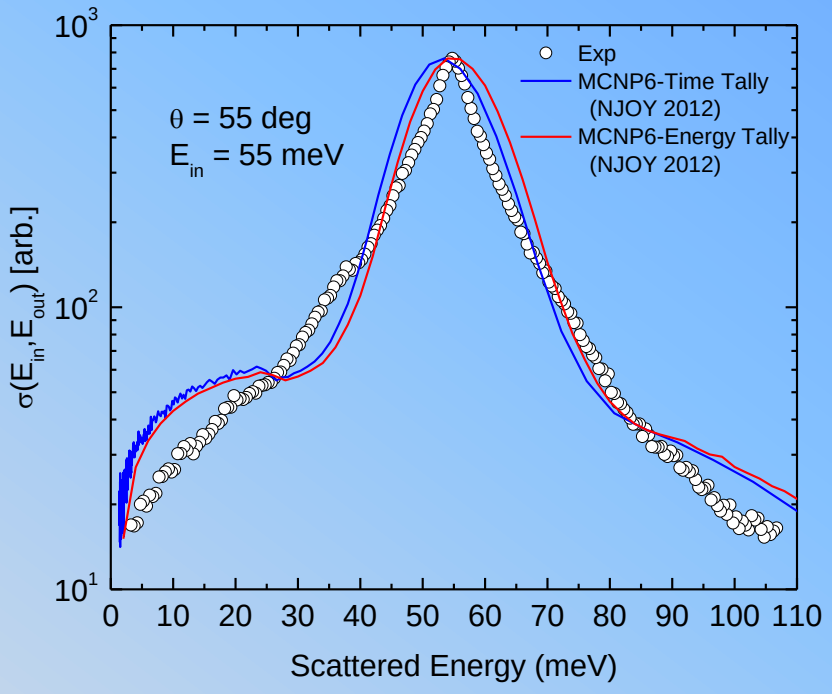
Thermal Scattering Overview

- Preformed measurements at SNS
  - SEQUOIA
    - Water
    - Medium Density Polyethylene (MDPE)
  - ARCS
    - High Density Polyethylene (HDPE) 295 °K and 5 °K
    - Quartz (SiO_2) at 20, 300 550, 600 °C
  - VISION (measures $S(\omega)$)
    - Lucite, Lexan, Polyethylene at 5 °K and 295 °K
- The double differential scattering data (DDSD) can be used to benchmark thermal scattering evaluations
- Method to generate $S(\alpha,\beta)$ from the experimental data are under development:
  1. Convert the data ($S(Q,\omega)$) to phonon spectrum (use low values of Q to limit multiple phonon scattering)
  2. Remove the elastic peak from the DDSD and convert the inelastic part directly to $S(\alpha,\beta)$
- Developed capabilities to use LAMMPS code to calculate the phonon spectrum and scattering kernel.

Scattering from Water

- For 160 meV incident energy where older RPI data exists:
  - The SNS experimental data is in agreement with the older RPI data
  - The simulation is in agreement with experiments
- For lower incident energy (55 meV) the simulation shows structure that is not visible in the data





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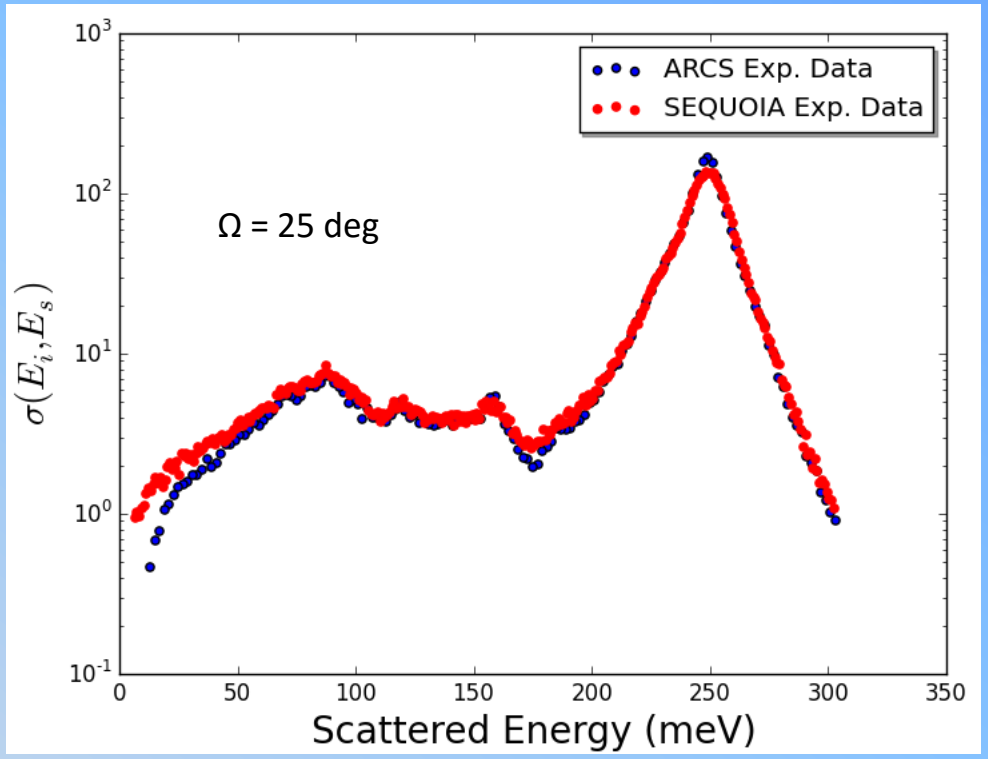
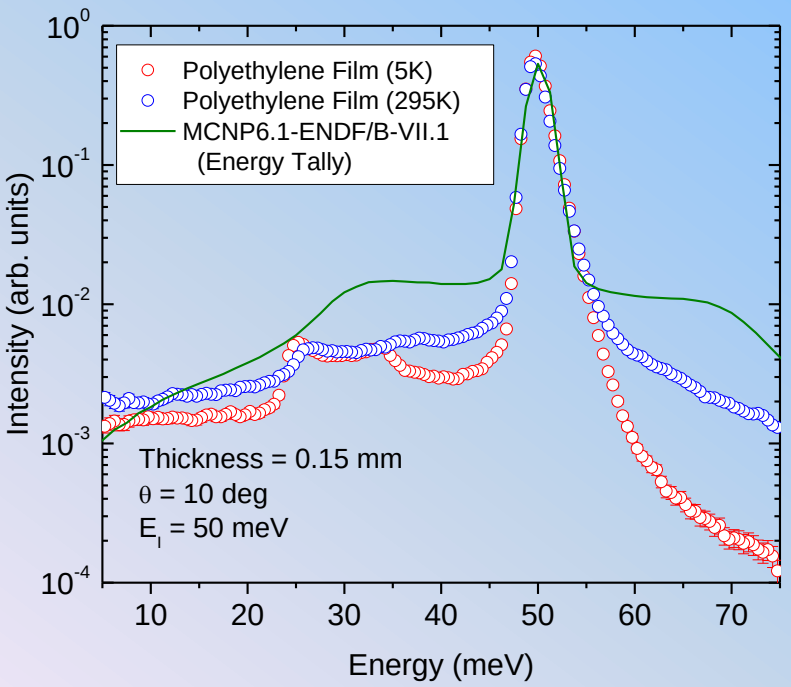
ARCS vs SEQUOIA

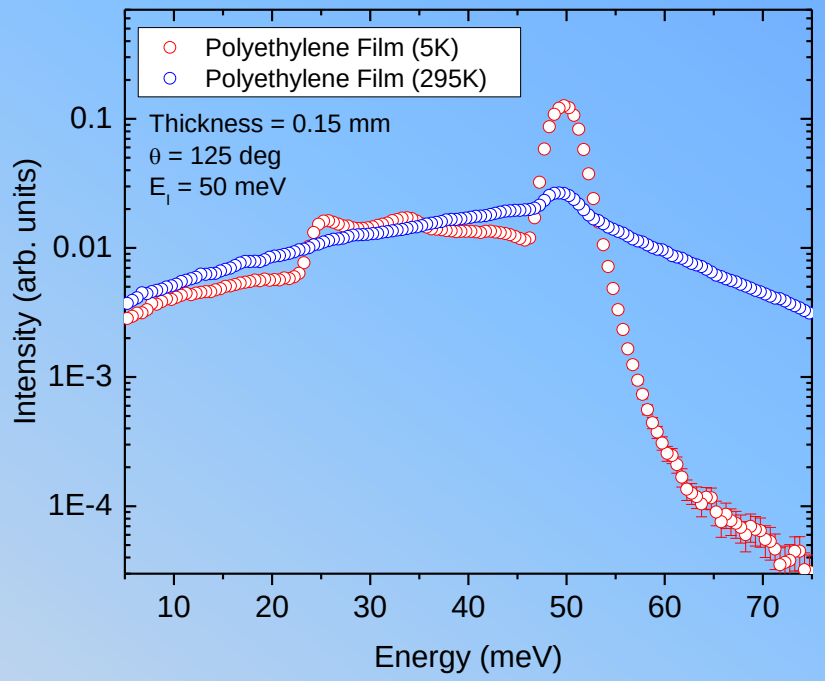
- 250 meV incident energy
- ARCS shows slightly better energy resolution compared to SEQUOIA
  - ARCS sample: CH_2 Sheets
  - SEQUOIA sample: CH_2 powder
- Sheets allow for coherent elastic scattering



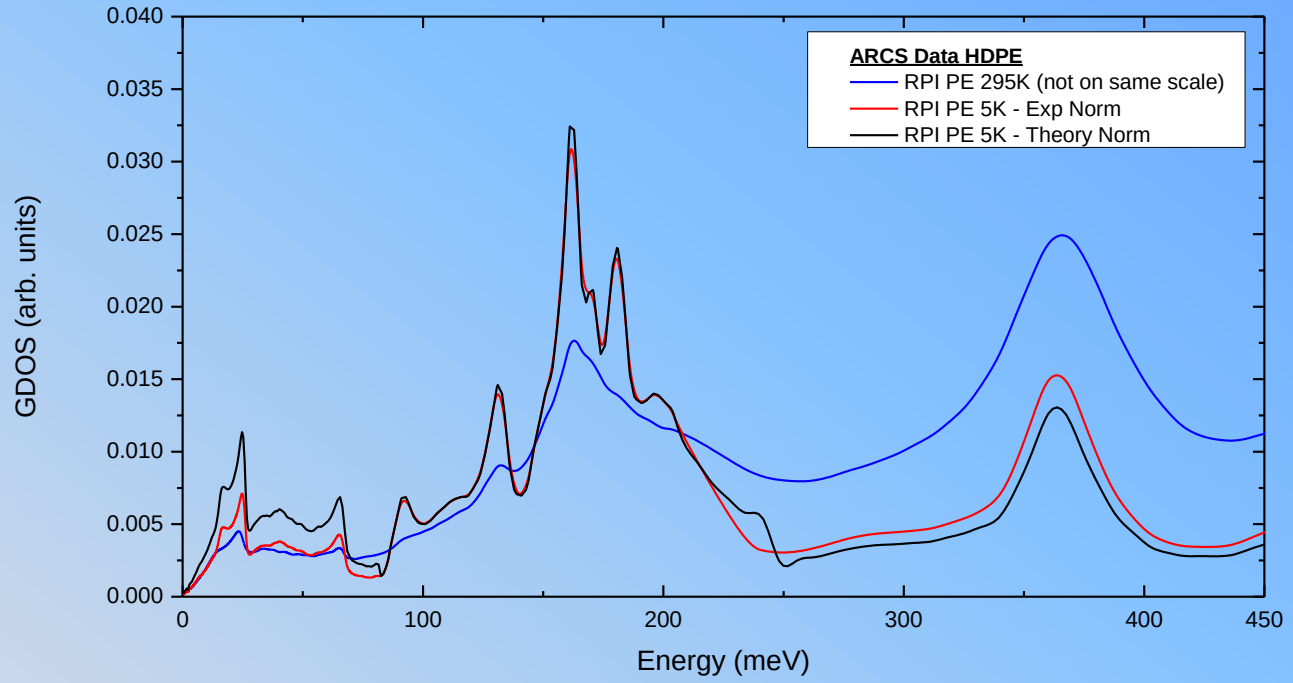
New Raw Experimental Data

- Polyethylene using ARCS-Wide Angle Spectrometer at SNS
- Low temperature reveals the vibrational/rotational modes





Phonon spectrum from measured $S(Q,E)$



- Low temperature measurements are essential in order to resolve the structure.
- Convert the measured $S(Q,E)$ data for phonon spectrum using the SNS DAVE code:

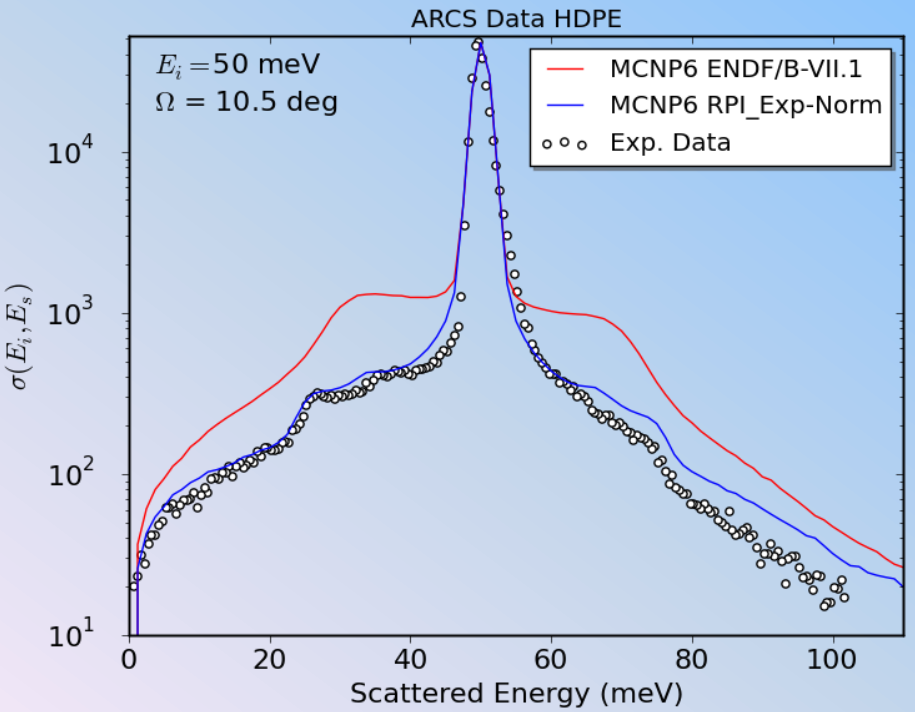
$$S(Q,E) = \frac{\hbar^2 Q^2}{6ME}\exp(-\langle u^2\rangle Q^2)G(E)[n(E,T)+1] \qquad n(E,T) = \frac{1}{\exp\left(\frac{E}{k_B T}\right)-1}$$

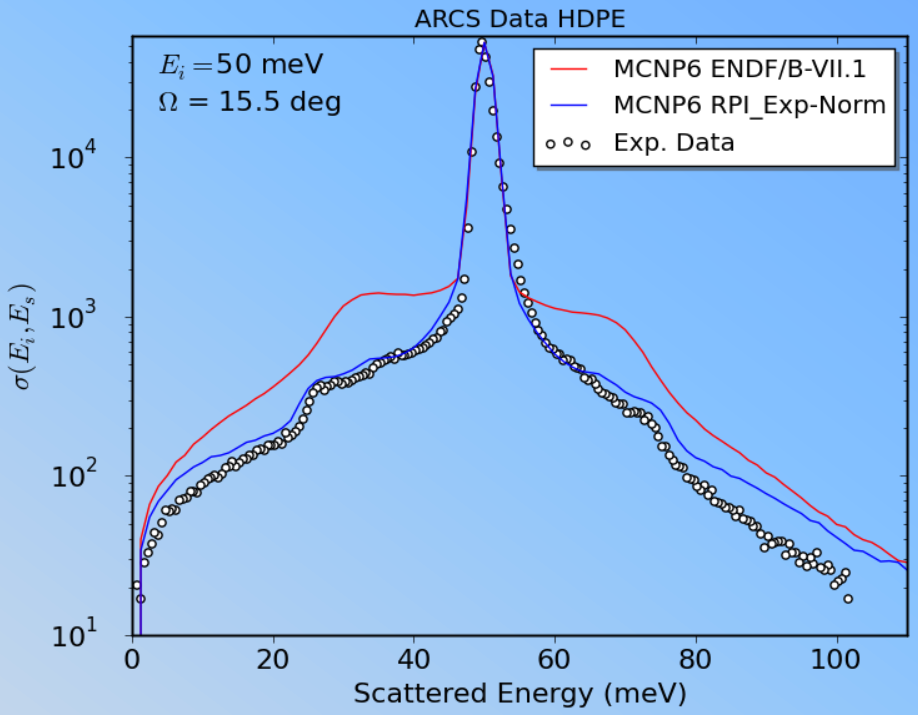
$G(E)$ - generalized phonon density-of-states(GDOS),
Q - wave vector transfer,
$S(Q,E)$ - structure dynamics factor,
M - mass of the atom,
$\langle u^2 \rangle$ - mean square displacement.

Example for HDPE

Experiment Normalized GDOS

- The phonon spectrum was processed with NJOY 2012
- The experimental response simulated with MCNP 6
- The agreement with the experiment is improved





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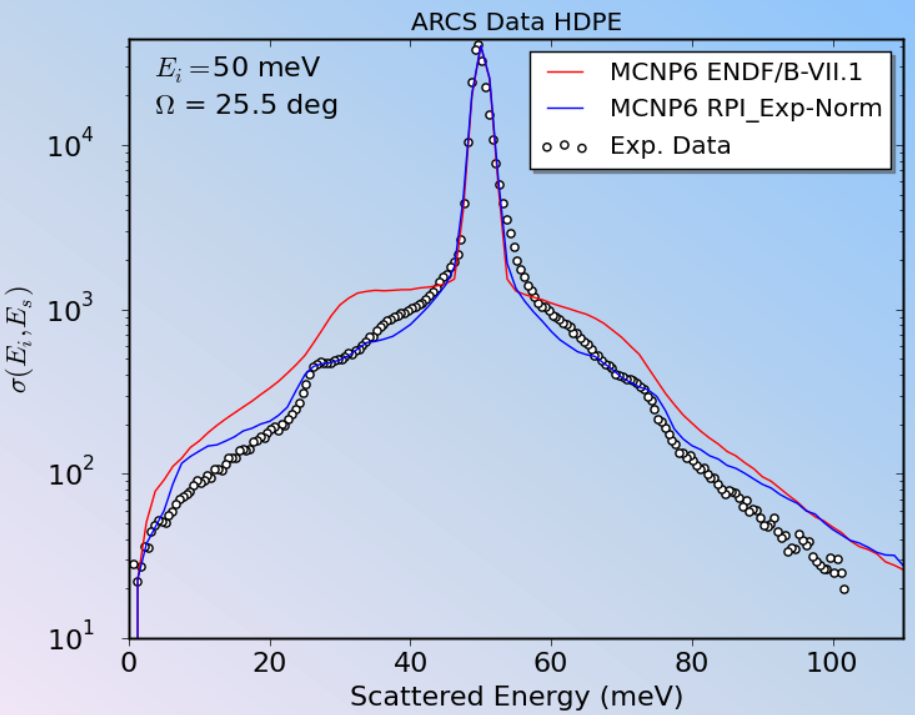
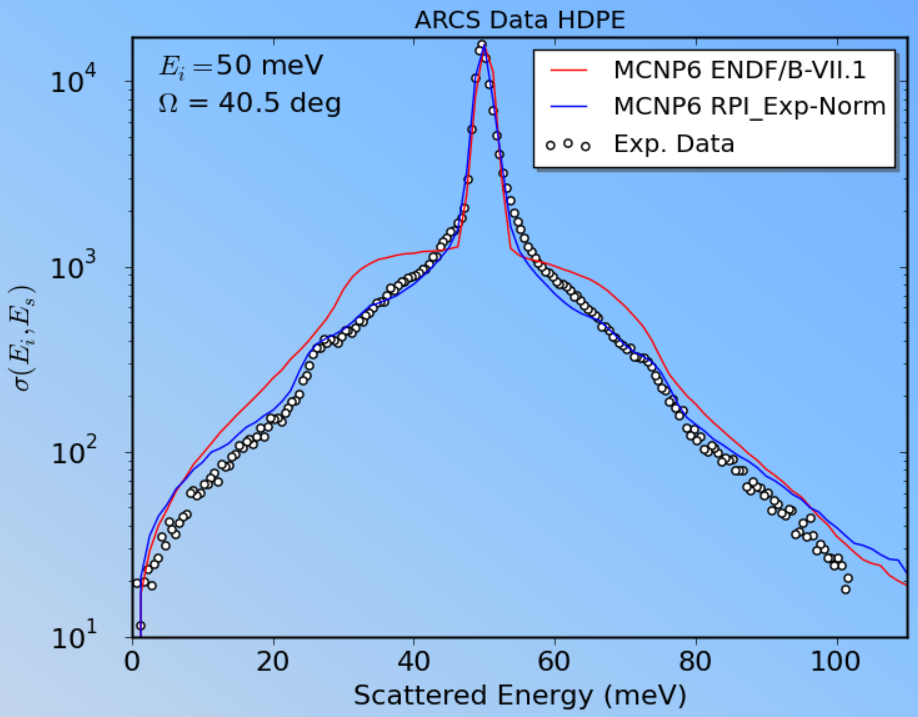
Example for HDPE other angles Experiment Normalized GDOS

- Similar improvements
- Other incident energies and angles available





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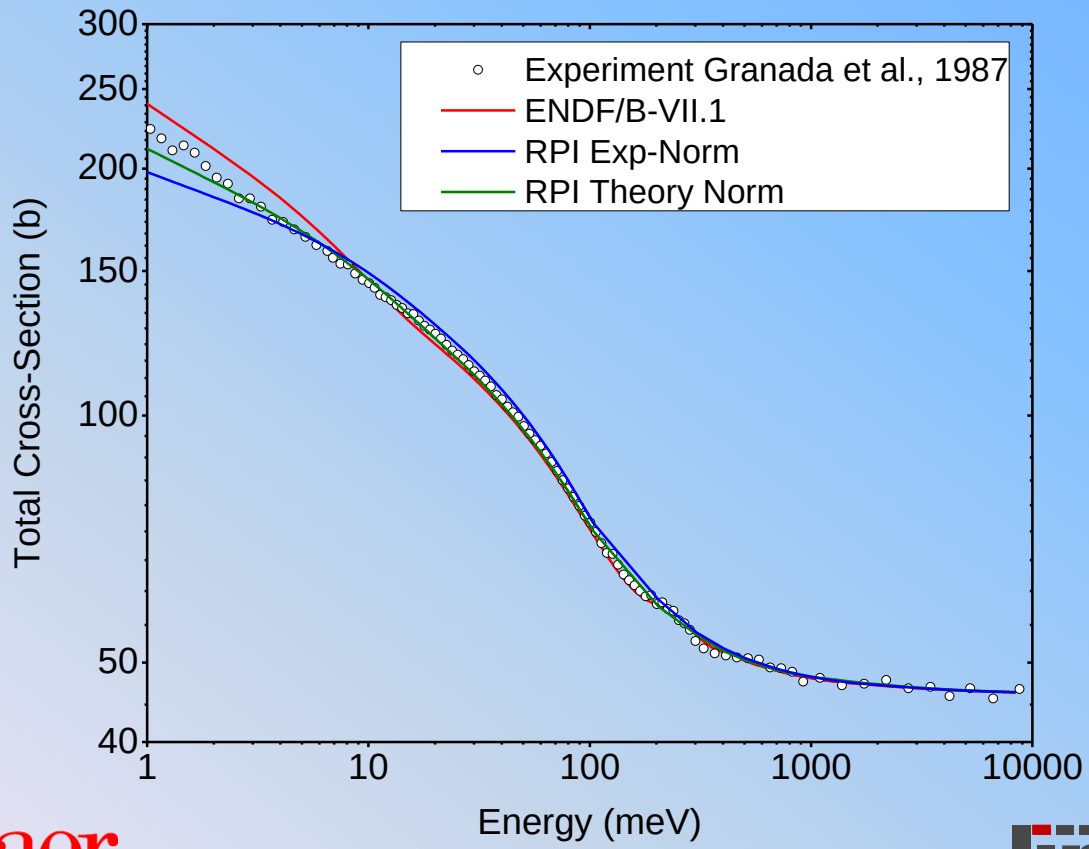
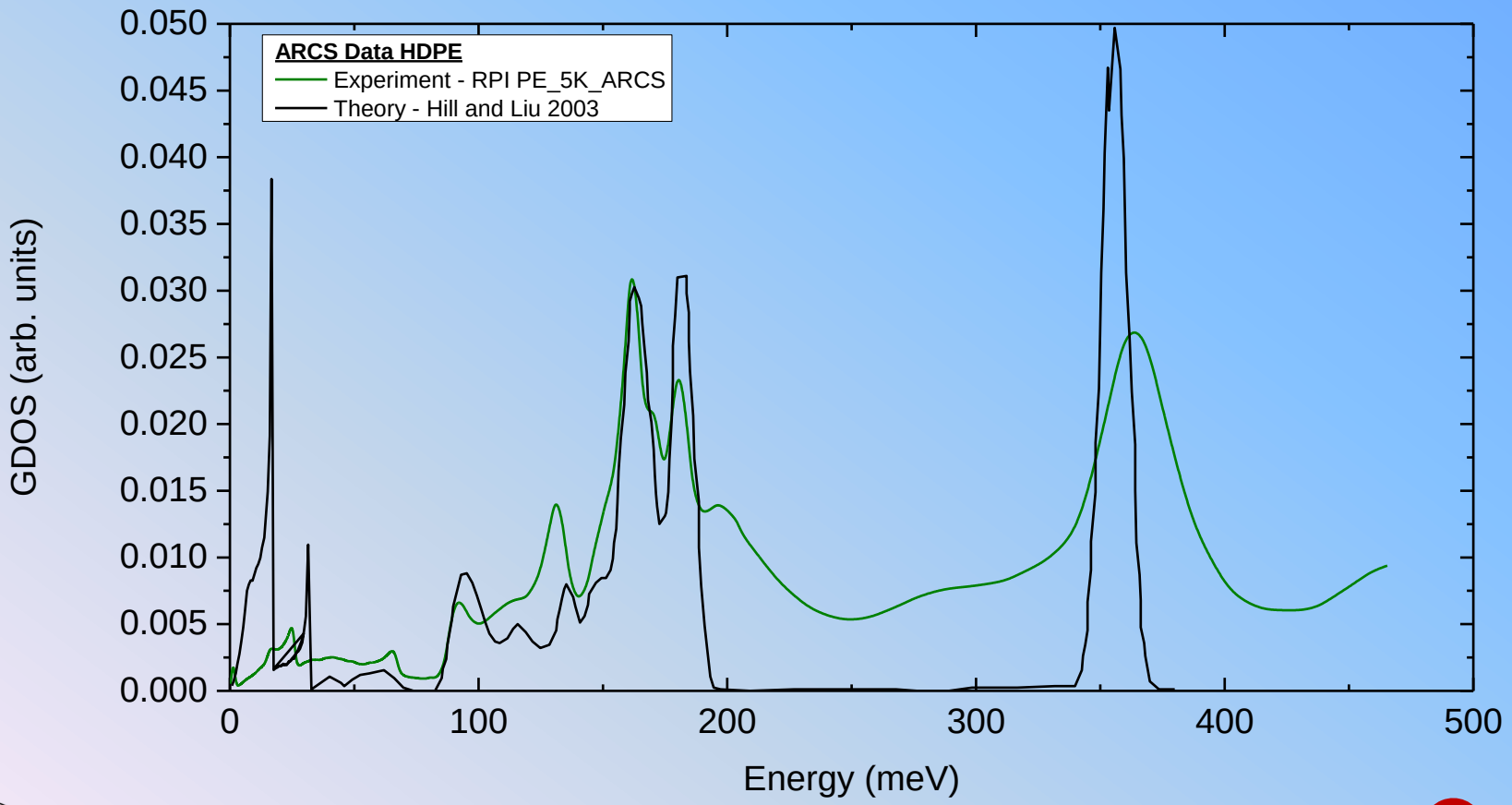
Polyethylene Total Cross Section

- The experimentally derived phonon spectrum is in good agreement with the total cross section measurement.
- The Experimental vs theory normalized measurement give slightly different results
  - Normalization to theoretical GDOS give better results (but this might be a unique case).



Theoretical GDOS

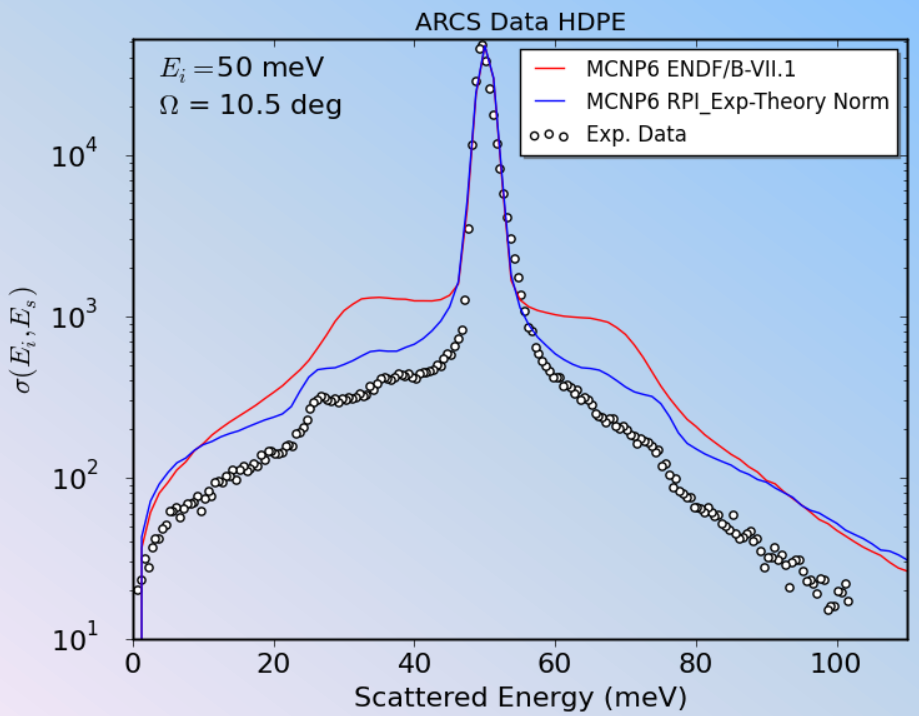
- Use theory to generate GDOS and use the peak rations to adjust the experimentally derived GDOS

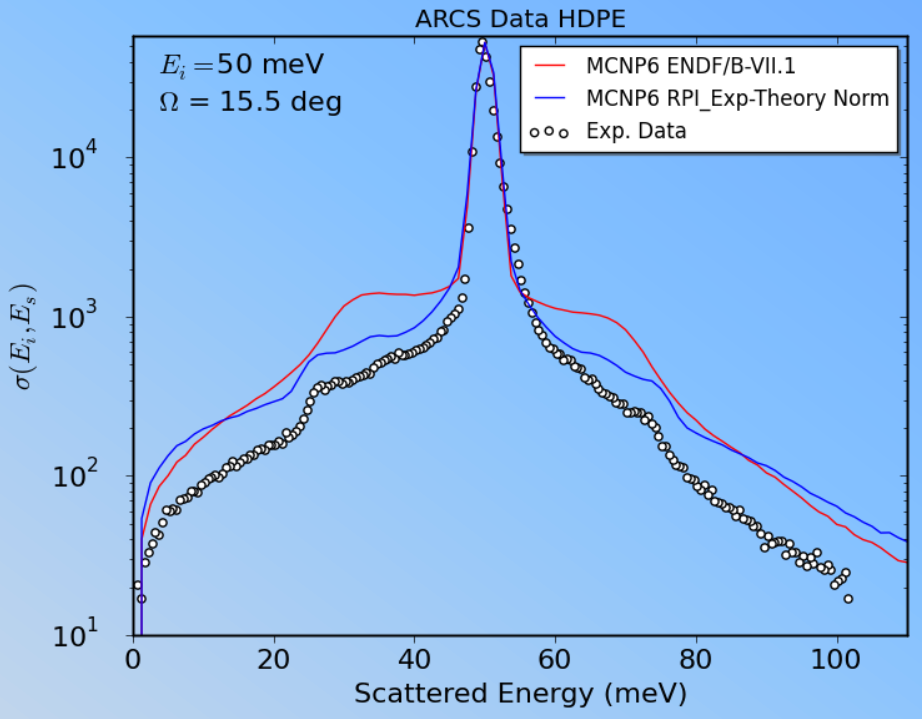


Example for HDPE

Theory Normalized GDOS

- Better agreement with total cross section but poorer agreement with double differential cross section.

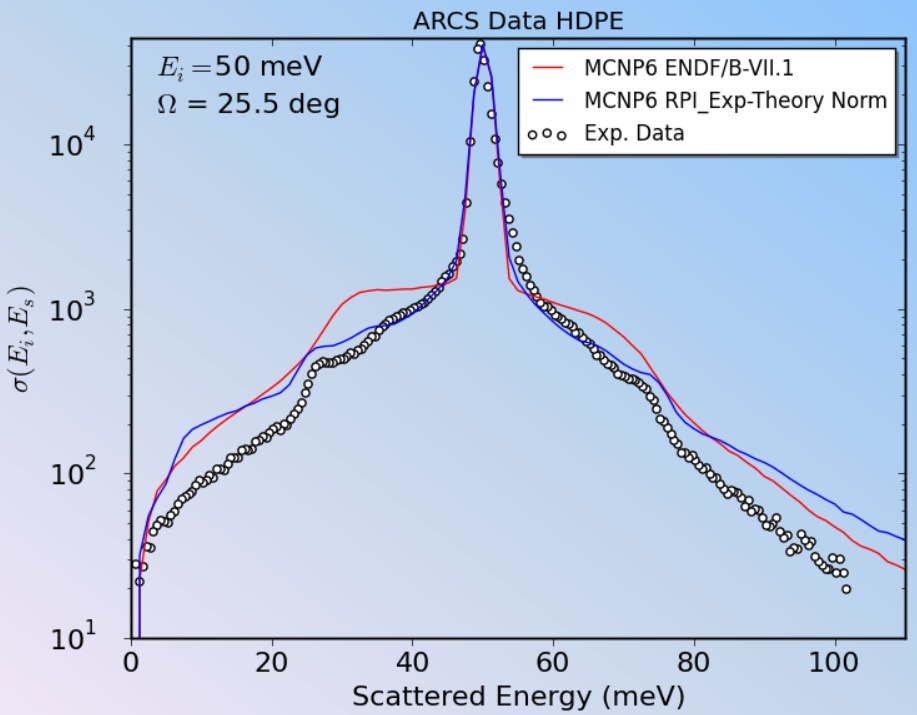


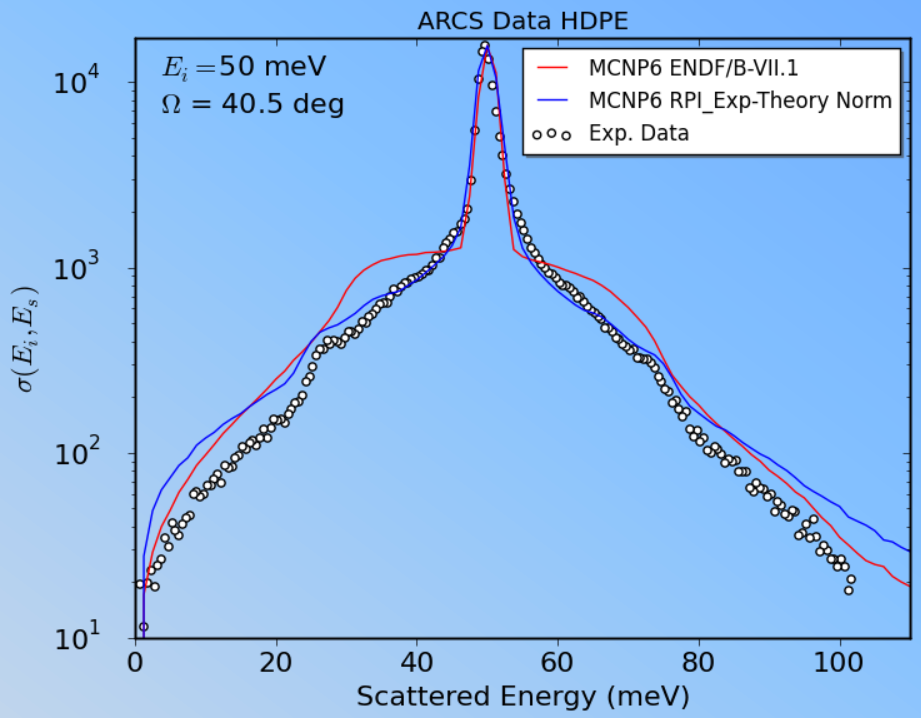


Example for HDPE other angles

Theory Normalized GDOS

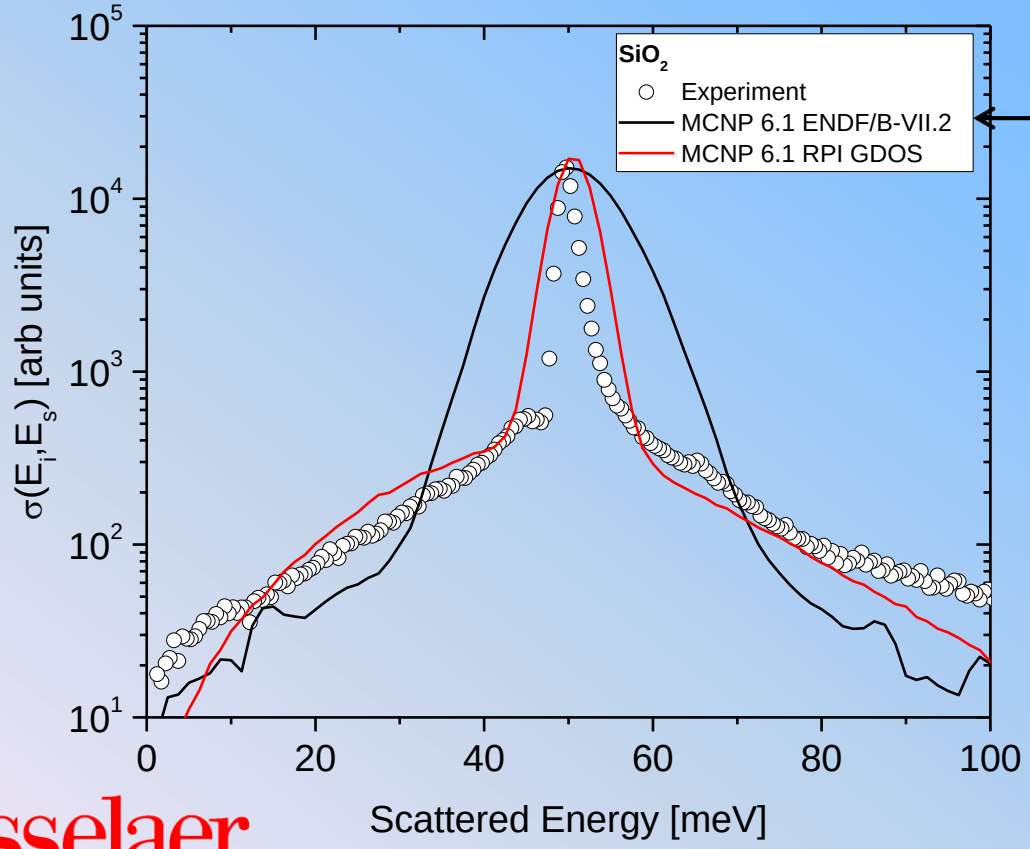
- Better agreement with total cross section but poorer agreement with double differential cross section.





ARCS Quartz Crystal

- SiO_2 was measured at multiple thicknesses
  - 0.3175 cm and 0.635 cm (1/8th and 1/4th inches)
  - Temperatures: 20º C, 300º C, 550º C, 600º C
- Experiment and simulation based on ENDF/B-VII.1 are not in good agreement
  - Are we measuring the same material that was evaluated?
- Preliminary experimental GDOS looks promising.



Indicates the updated quartz evaluation

Summary

- **Measurements (at SNS)**
  - Difficult to get beam time but possible.
  - Completed for H_2O, Polyethylene, Quartz, (Lucite, Lexan, Polyethylene on VISION)
- **Thermal double differential data can be used:**
  - To validate thermal scattering evaluations
  - To improve thermal scattering evaluations
- **Two methods for experiment based evaluations**
  1. Derive phonon spectrum from double differential scattering experiment
     - Measurements at 5 K were helpful
  2. Direct conversion of measurement to $S(\alpha,\beta)$ is still under development
  - Need accurate total cross sections (can be done at RPI)
- Need to complete evaluations for all measured materials and perform critical benchmark calculations.