Experimental Nuclear Data Program at the Gaerttner LINAC Center at RPI

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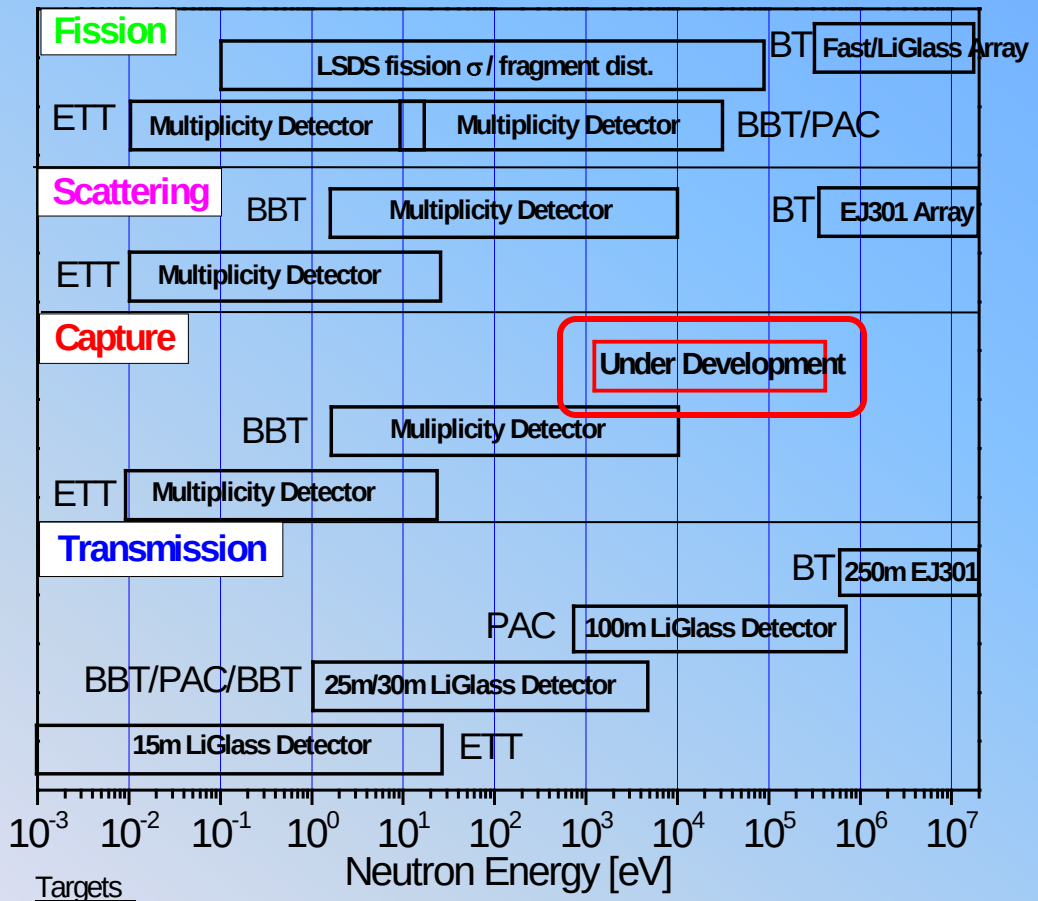
Overview

- **ND-1- Resonance Region Nuclear Data Measurement**
  - Development of a new mid energy capture detector
    - 45m flight path, energy range from 1 keV to 500 keV
    - Performed measurements of Fe and $^{92/94}$Mo
  - Transmission measurement of ^{186}W at 35m
    - In support of ORNL ND task
  - Neutron scattering measurements for ^{56}Fe
    - 30m flight path, 0.5 MeV to 20 MeV
    - Obtained the ratio of inelastic to 1st state to elastic scattering.
- **ND-2 Thermal Neutron Scattering Measurements**
  - Performed analysis of previously measured samples of water and medium density polyethylene.
  - Measured neutron scattering from samples of quartz (SiO_2) and High Density Polyethylene (HDPE) at several temperatures.
- **ND-3 LINAC 2020 Refurbishment and Upgrade Plan**
  - Project started, klystron order expected in FY-14

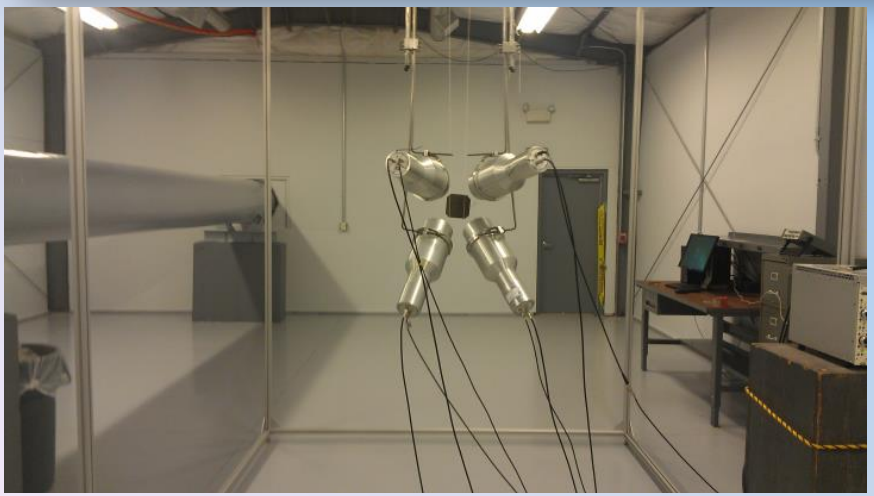
Capability Development

- Develop Mid energy (1 - 500 keV) capture detector



Targets
ETT- Enhanced Thermal Traget
BBT - Bare Bounce Target
BT- Bare Target on Axis
PAC - PacMan Target

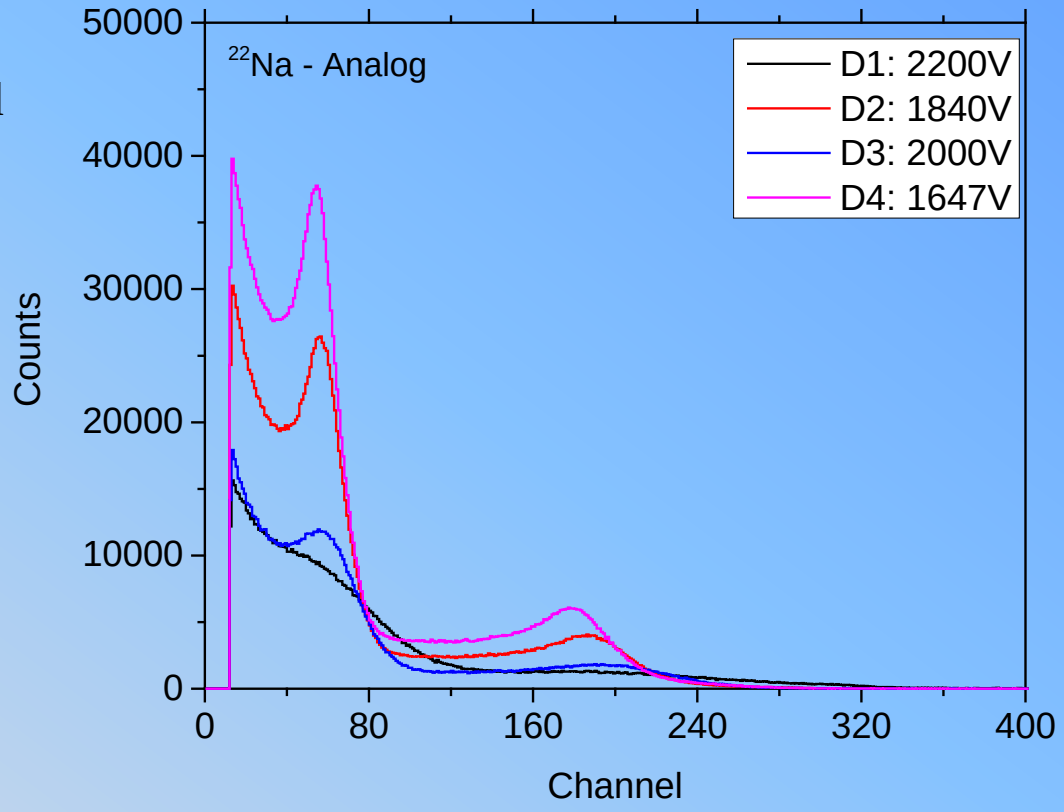
New Flight Station and Capture Detector



- Flight Station construction completed in FY 12
- FY 13
  - Installed capture detector array
  - Installed evacuated flight tubes
  - Installed sample changer
  - Performed a test run with Fe
- FY 14
  - Resolving issues with two detectors (sent back to Eljen)
  - Performed a scoping measurement of Fe and $^{92/94}$Mo

Mid-Energy Capture Detector

- Two detector modules exhibited poor energy resolution and pulse shape
- Modules were returned to vendor for repair and fitting with new PMTs
- Expected return date: April, 1, 2014
- Scoping experiment performed with 2 remaining detectors

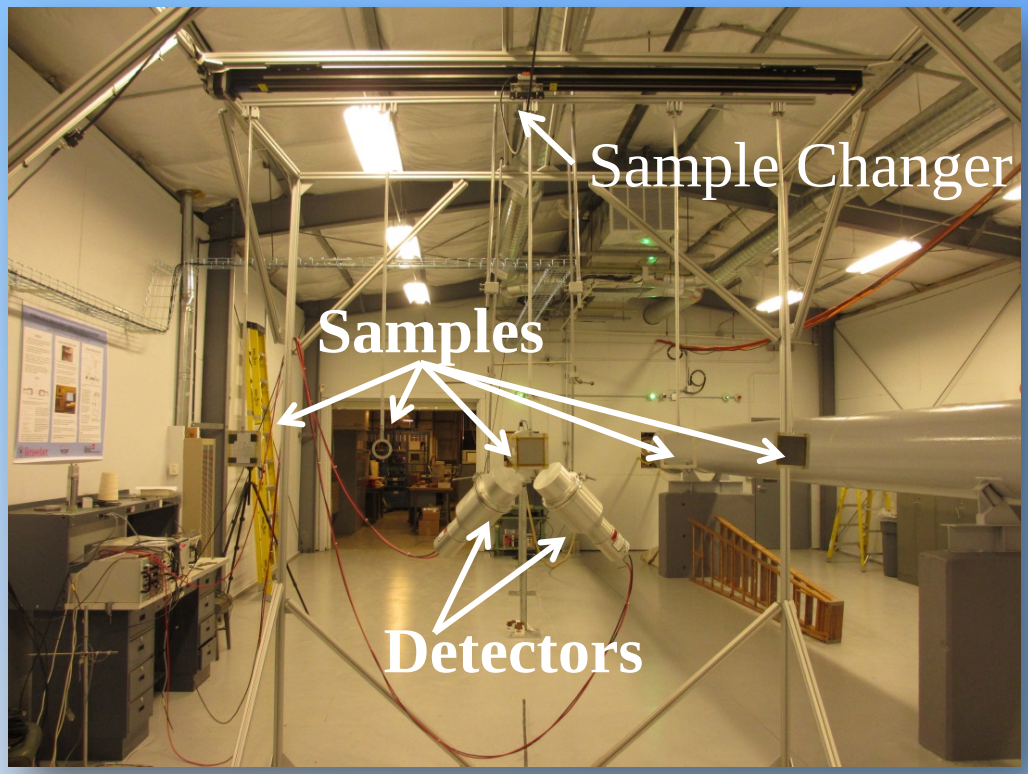


MCA spectra of 4 detector modules with detectors 1 and 3 showing degraded performance

Mid-Energy Capture Detector
Sample Changer

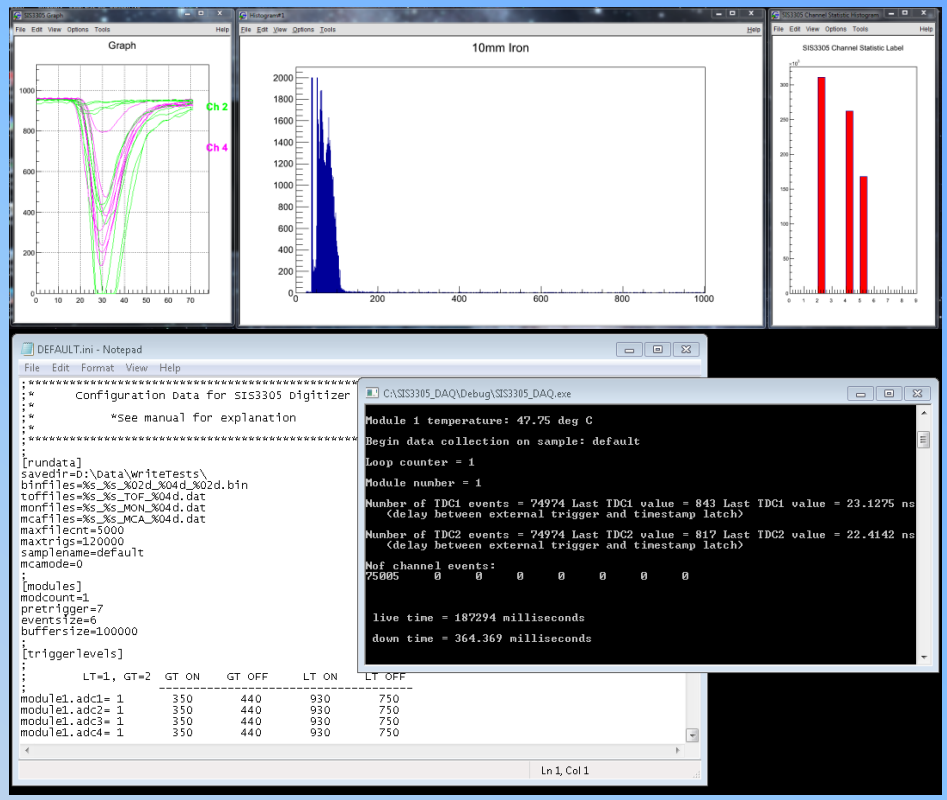
- Ceiling-mounted sample changer
- 84” Velmex BiSlide linear translation module with stepper motor
- Linear magnetic encoder for micron-precision sample position verification
- Customizable with up to 5 samples of varying shapes and sizes
- Lightweight aluminum construction
- Computer controllable through LabView, with custom control software under development

- **Flight path was 45m**



Mid-Energy Capture Detector - DAQ

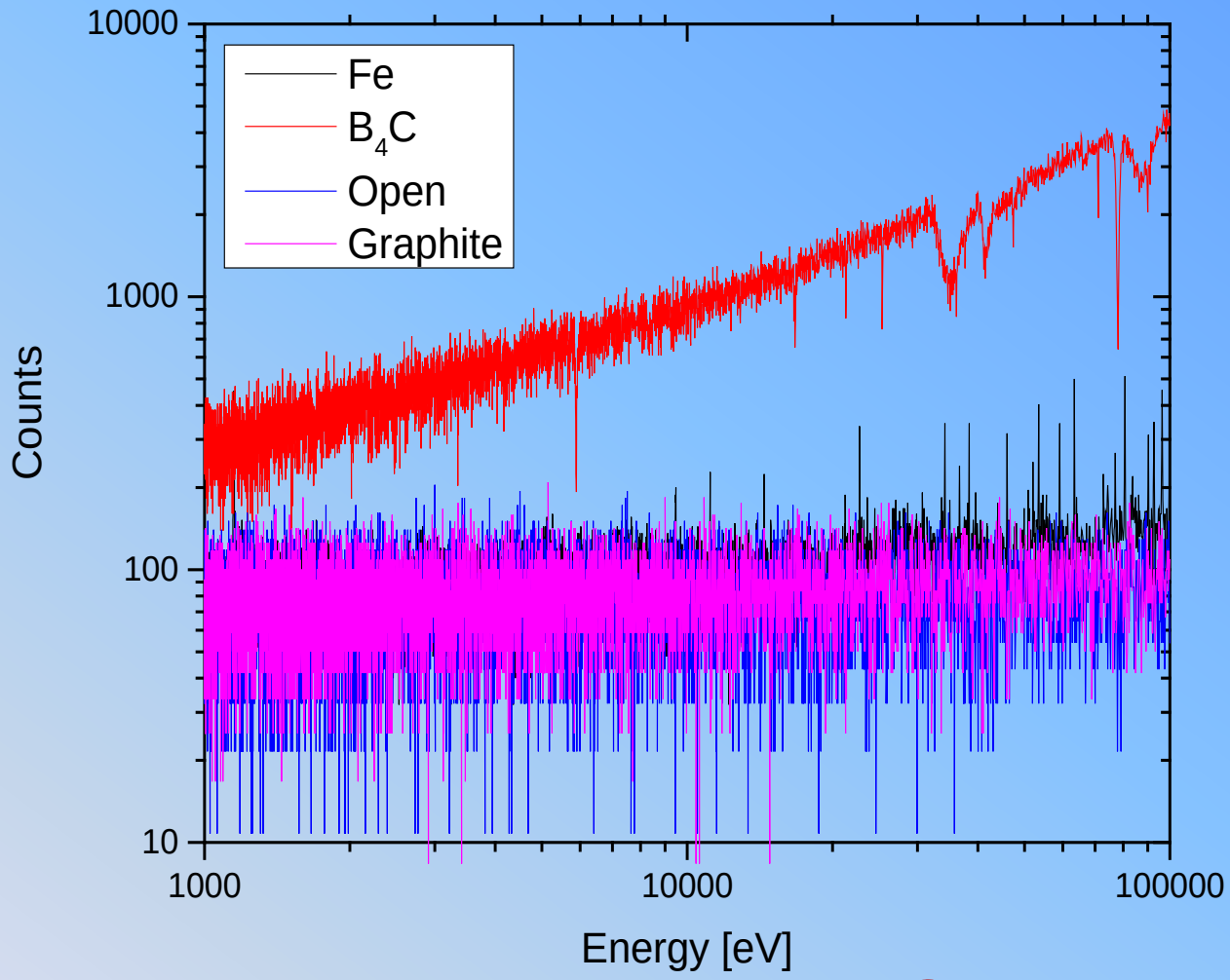
- Updated DAQ software for 10-bit, 1.25GHz SIS3305 digitizer
- Expandable to 8 DAQ boards with 8 channels each, for a total of 64 possible detector channels
- Buffered data transfer with real-time data streaming option under development
- Data collection paused during buffer transfer, <2% down time
- On-line plotting feature available using CERN ROOT libraries



Screenshots of DAQ software in operation

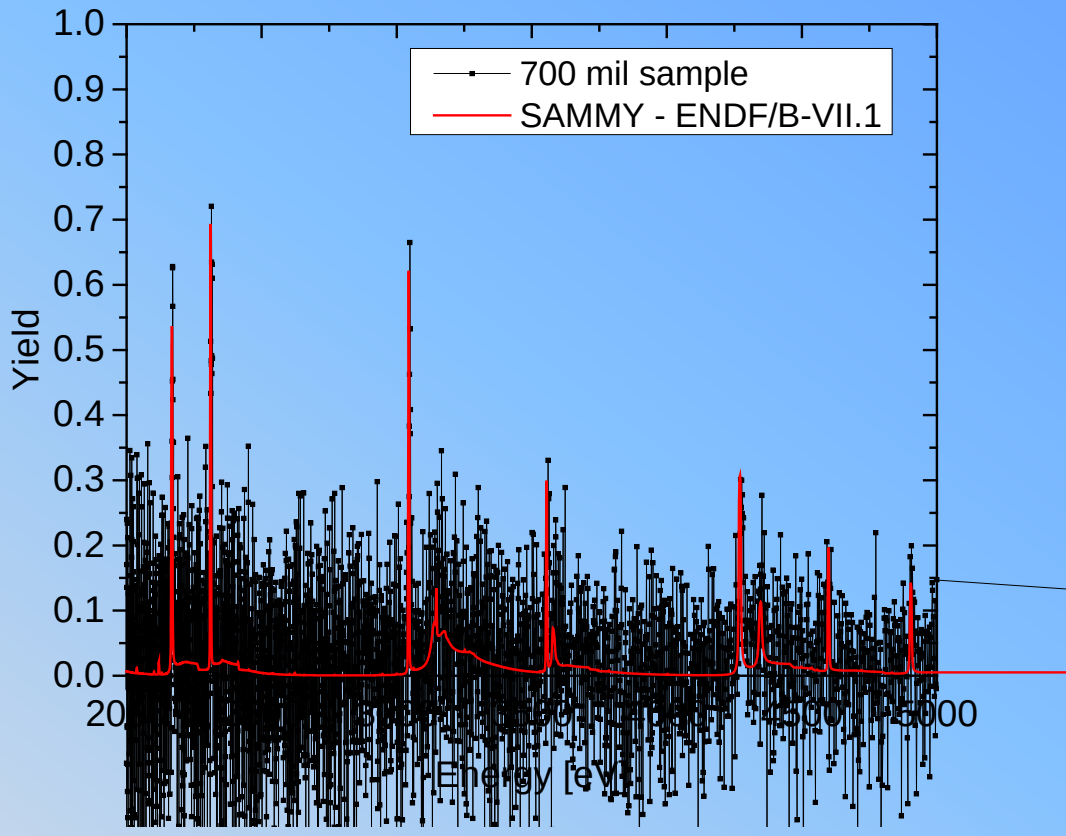
Raw Data for Fe capture experiment

- Used 2 C_6D_6 Detectors
- Data was grouped to 16 ns bins
- Neutron count rate is increasing with energy.
- Graphite sample was used to assess the neutron sensitivity
  - Graphite counts are art background level (open)
  - Longer measurement is needed to assess the scattering-to-capture ratio



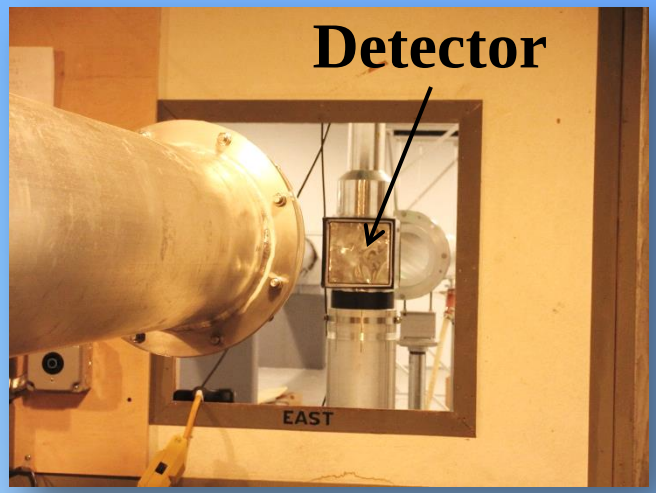
Scoping experiment for capture on $^{92/94}$Mo

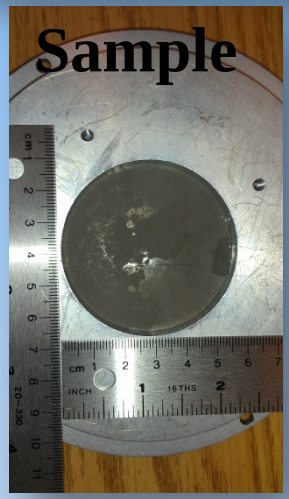
- Mo capture is one of the tasks for FY-14
- Enriched Mo samples were prepared by Bettis Atomic Power Lab (75.63% ^{92}Mo, 23.78% ^{94}Mo)
- For this scoping analysis data was grouped to 8 ns bins
- Samples were also measured in transmission at 100m flight path.
  - An energy shift was observed in both measurements which indicates a possible error in ENDF
- The sample yield is low, a thicker sample might be needed for higher energies where the yield is lower



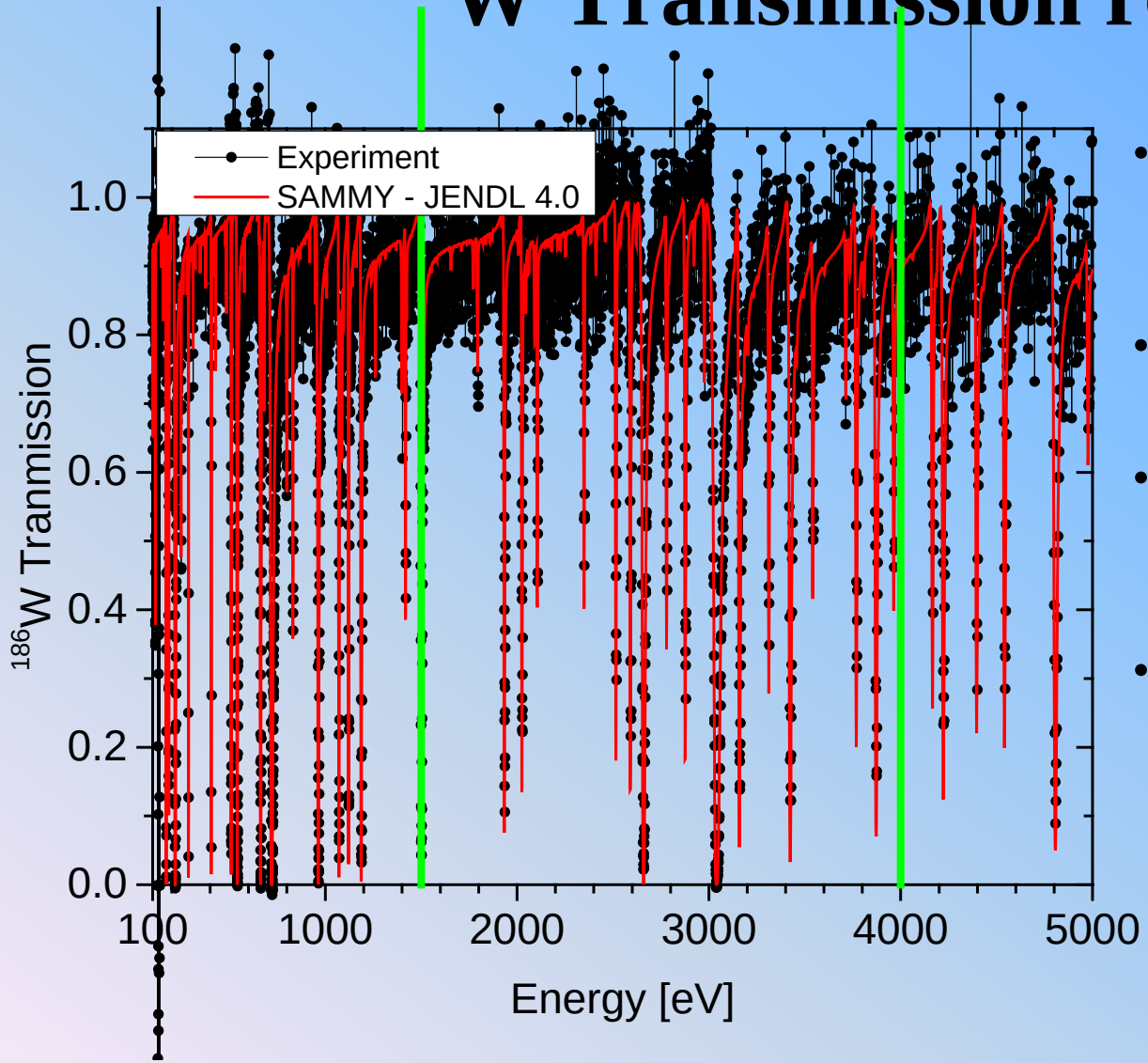
Transmission of ^{186}W

- Experiment was designed to provide data in the energy range from about 2-4 keV (Na fixed filter at Geel)
- Sample provided by ORNL
  - 3 discs, 0.01169 atoms/barn
  - ^{238}U sample for determination of the energy resolution
- Data was collected for 3.5 days.
  - 35 m flight path
  - Pulse width of 10 ns
- Co and Al fixed notches were used for background determination





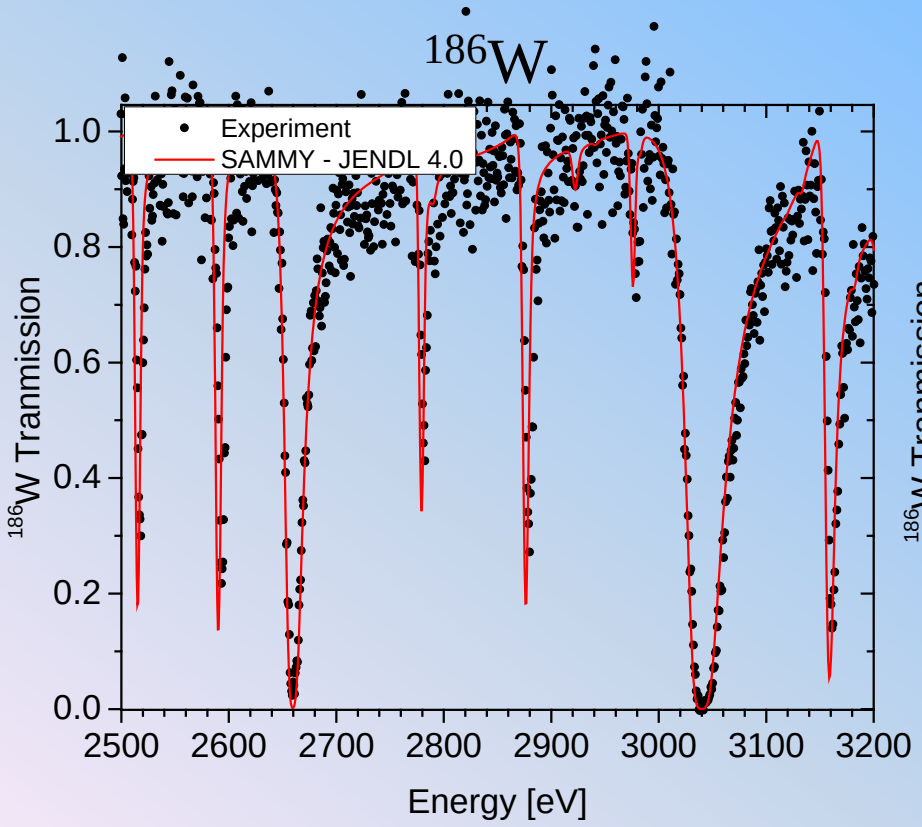
^{186}W Transmission results

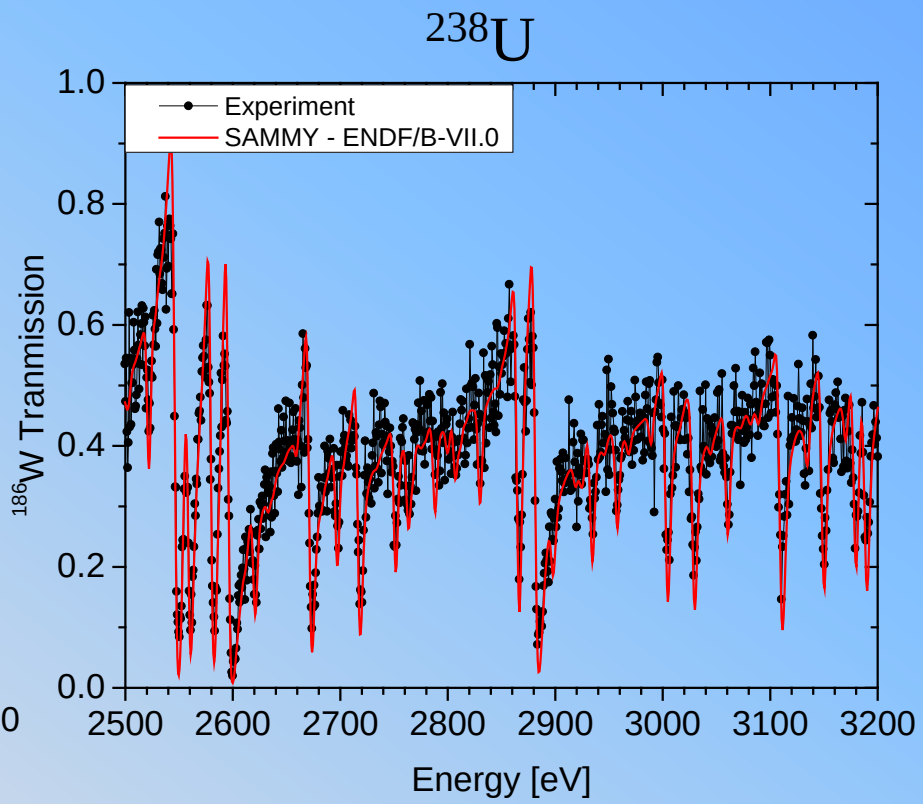


- Transmission measured covers the energy range from a 10 eV to 400 keV
- The region of interest is highlighted in green
- On this scale seems like goo agreement with JENDL 4.0
- ENDF/B-VII.1 seemed to have some issue with extra resonances.

^{186}W Transmission results: 2.5 – 3.2 keV

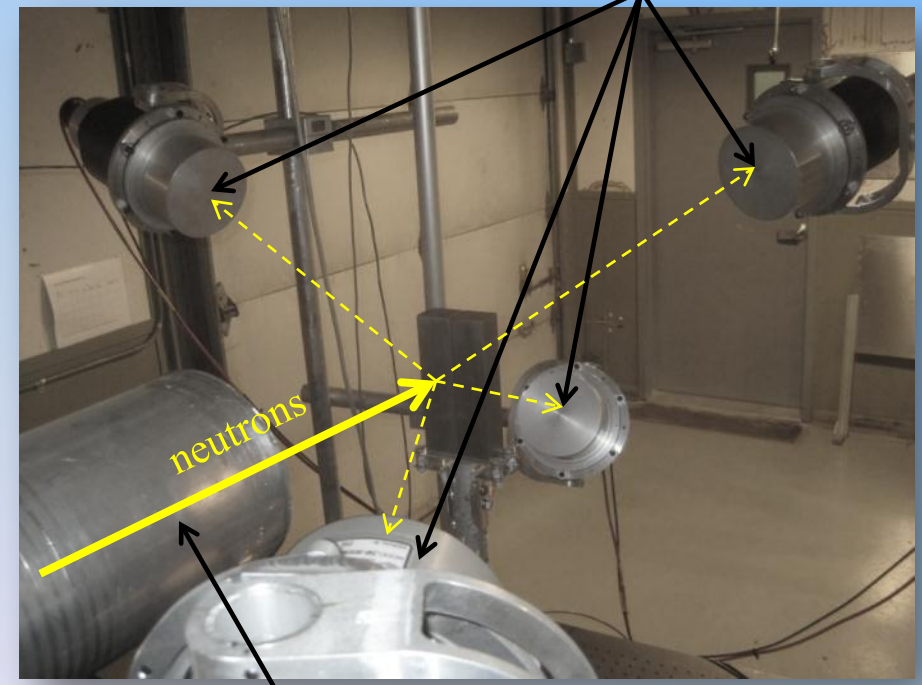
- Energy resolution was fitted to the ^{238}U sample
- ^{186}W shows energy shift which are not visible in the ^{238}U
- Preliminary data was delivered to ORNL





^{56}Fe Scattering Measurement - Setup

EJ-301 Liquid Scintillator Neutron Detectors



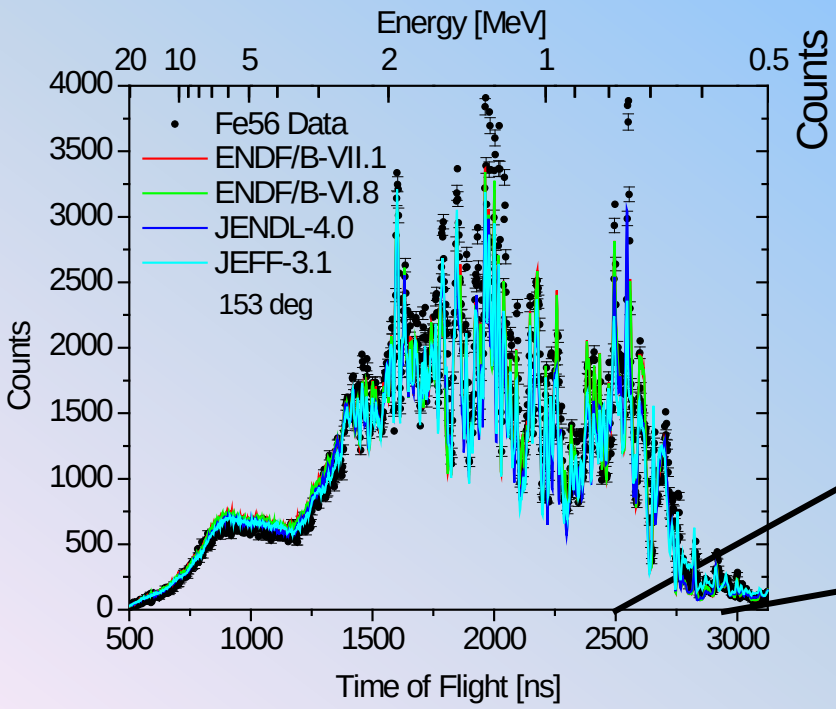
Evacuated Flight Tube

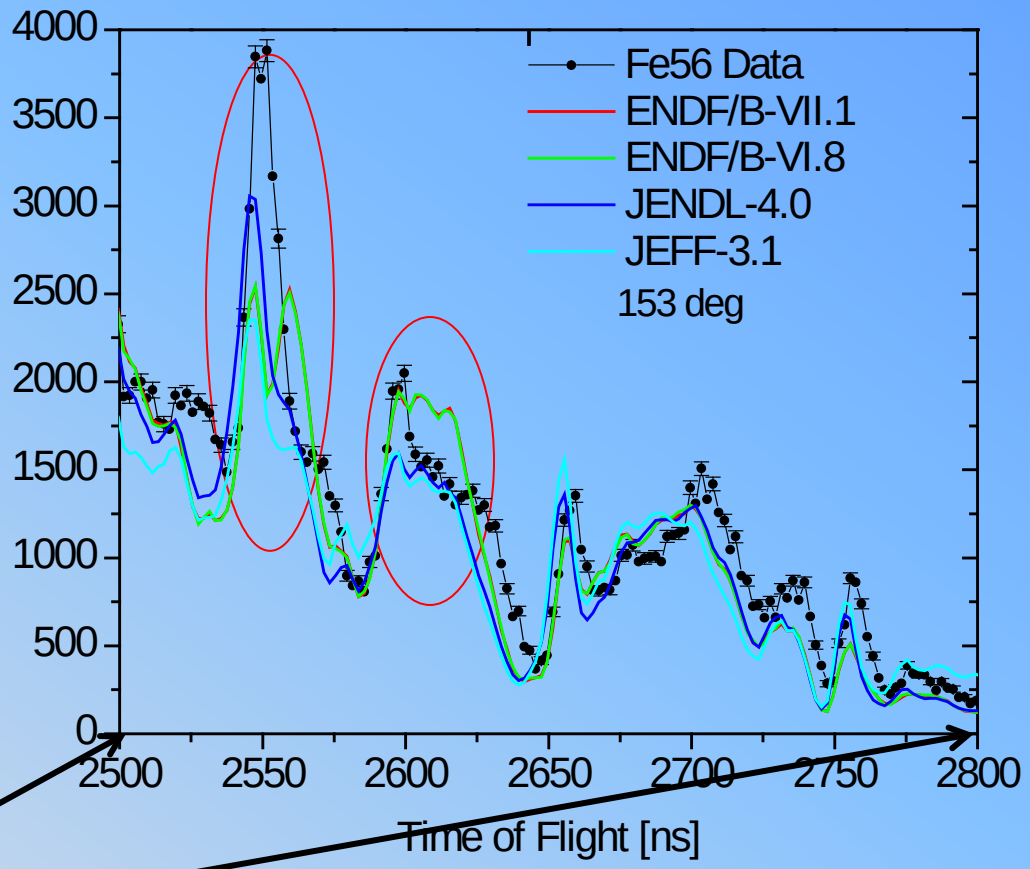
- ^{56}Fe Sample
- 99.87% metallic ^{56}Fe
- Dimensions 77.0 x 152.6 x 32.2 mm

The neutron beam size is smaller than the sample.

^{56}Fe Scattering Measurement – Results 153°

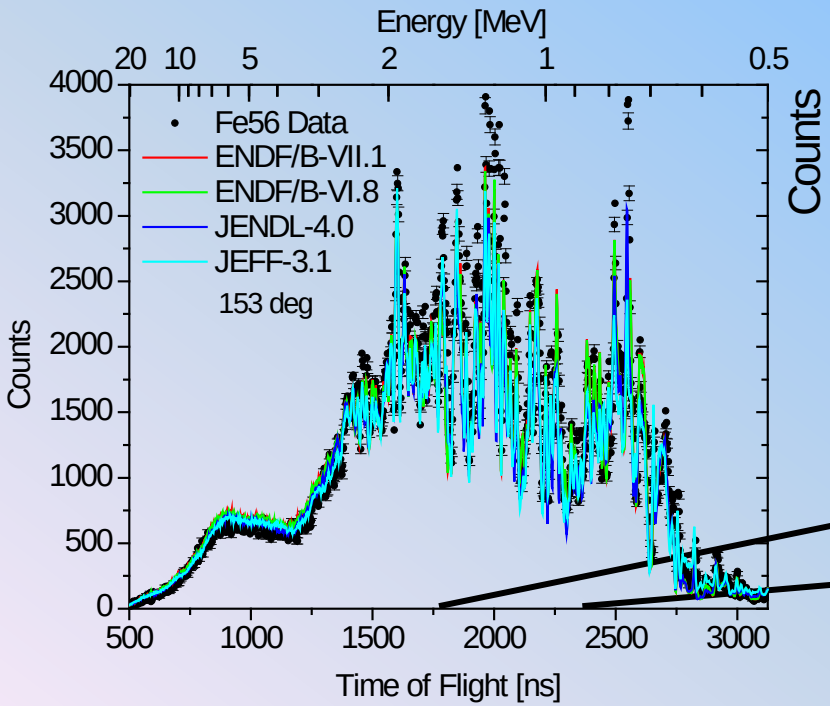
The energy resolution is sufficient to show some discrepancies in the resonance region (E<850 keV)

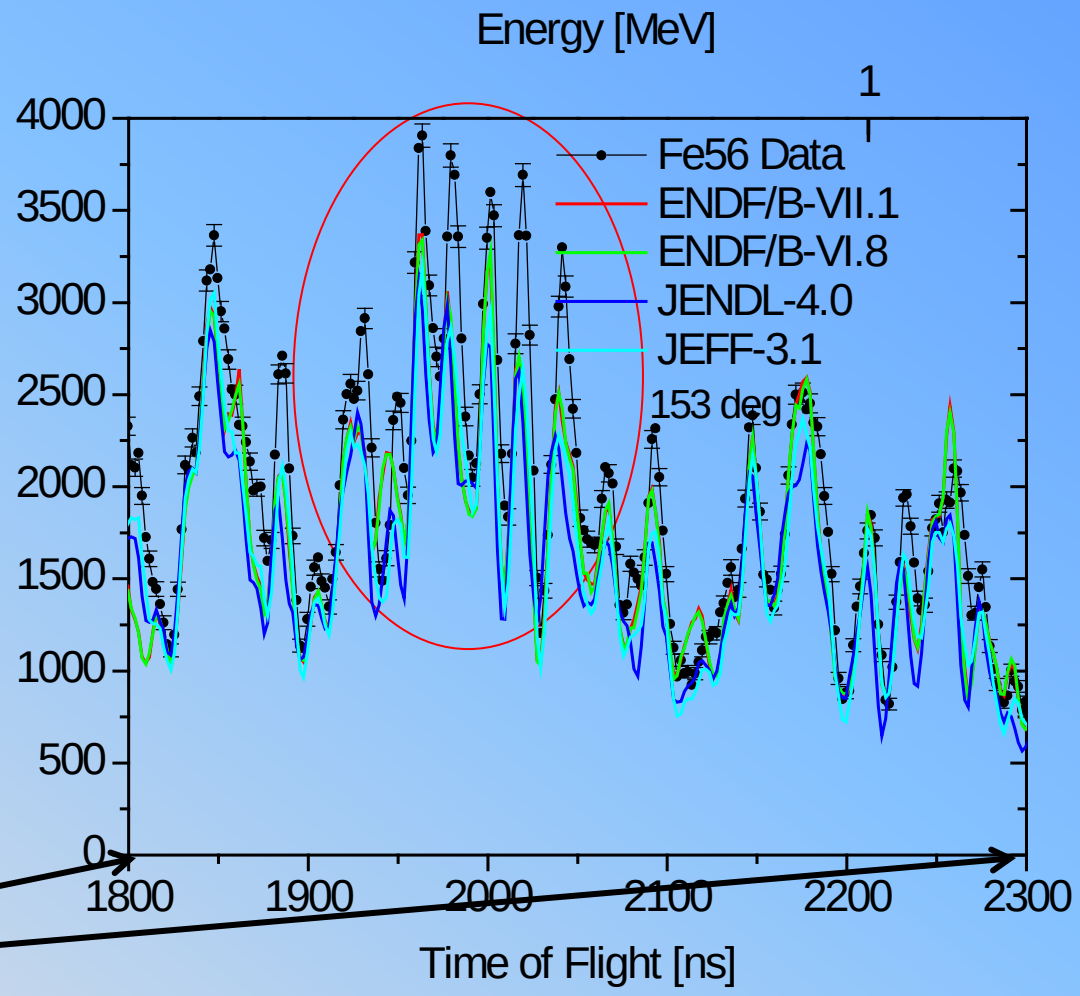




Fe-56 Scattering Measurement – Results 153°

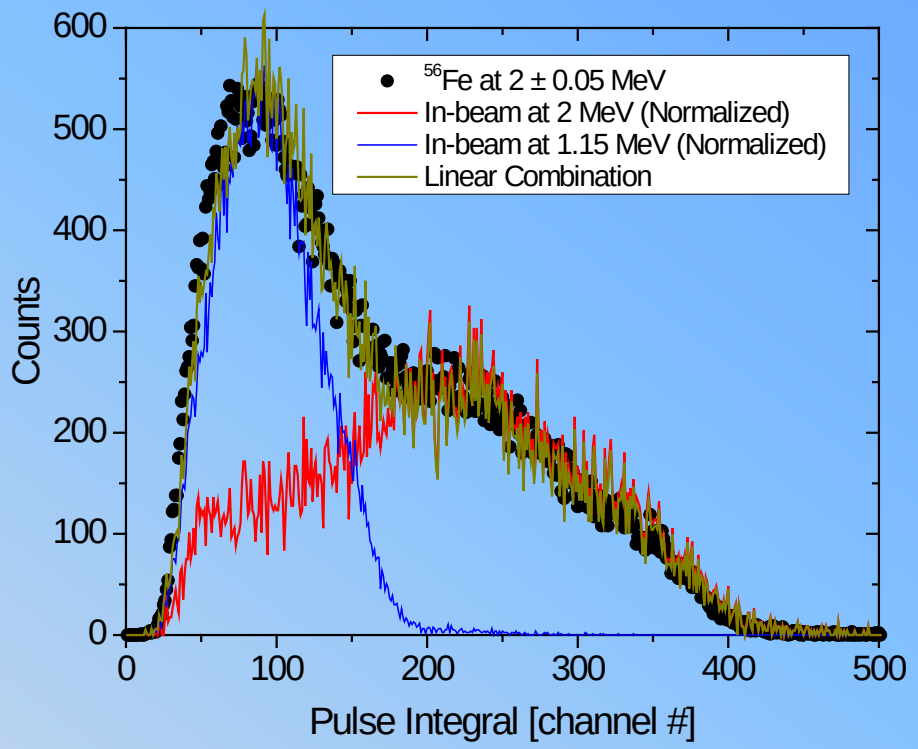
- Above the first inelastic state (E>847 keV) there are some differences with the evaluations
- We are exploring the possibility to extract double differential cross section data from these experiments.





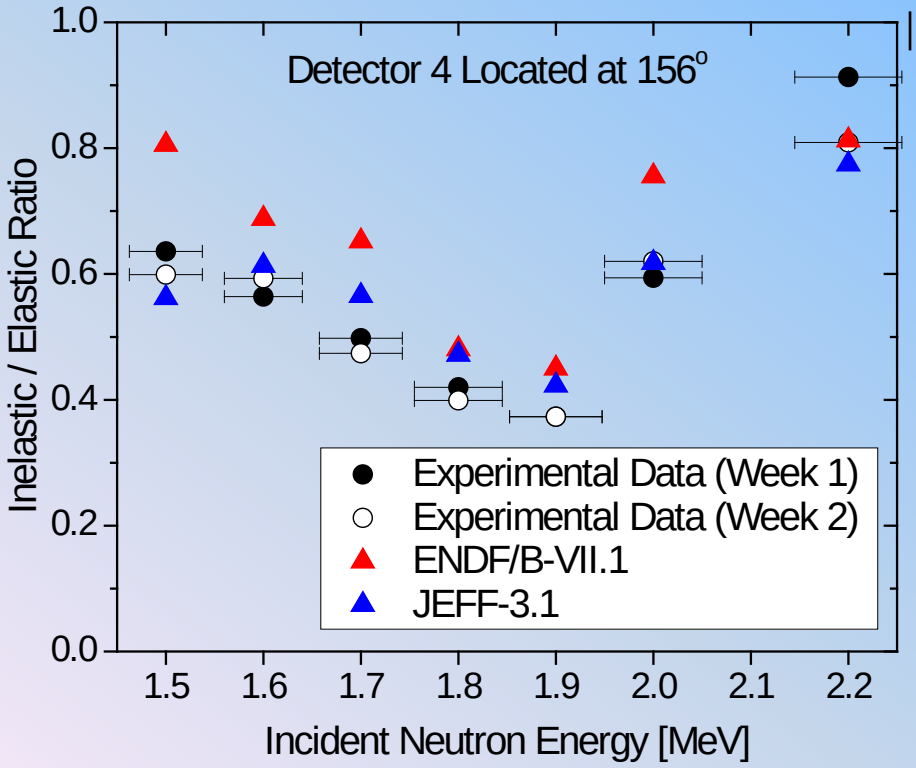
Elastic to Inelastic Scattering Ratio: Data

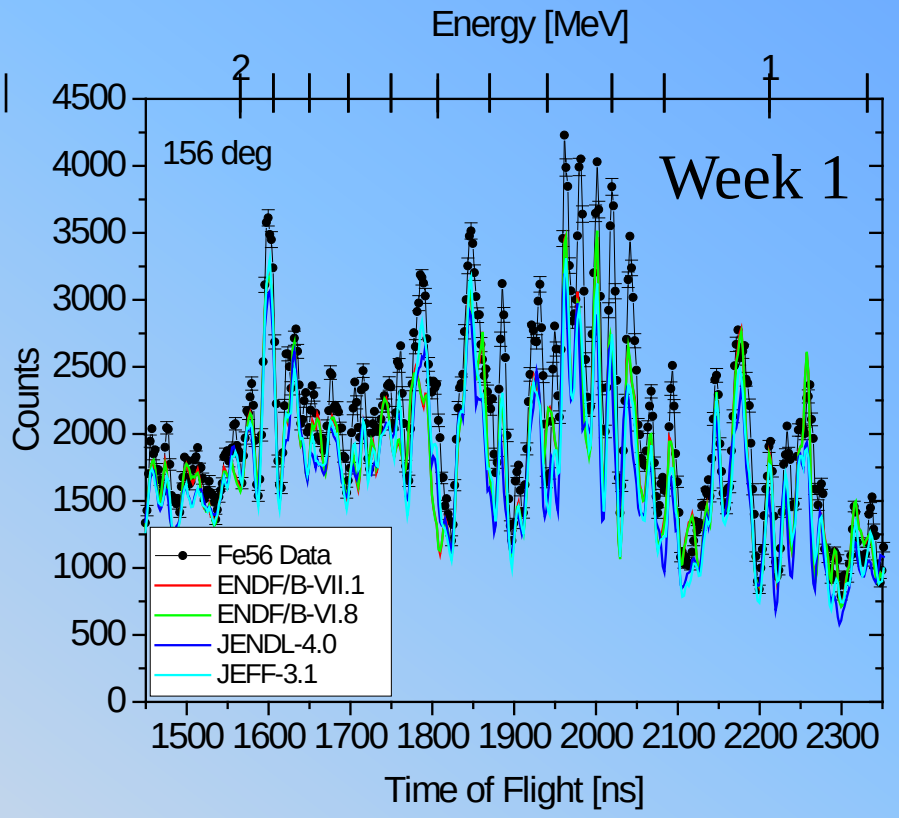
- ^{56}Fe scattering measured data for E_n>1.3 MeV includes elastic and inelastic neutrons
  - We can measure scattered neutrons when E_n>0.5 MeV
- The energy deposition by inelastically scattered neutrons is much lower than that of elastically scattered neutrons (by ~0.847 MeV depending on the scattering angle)
- The pulse height spectrum collected over a narrow neutron time of flight range corresponding to a certain incident neutron energy enables separation the two contributions.



1St Inelastic to Scattering Ratio at 156 deg Experiment and Evaluations

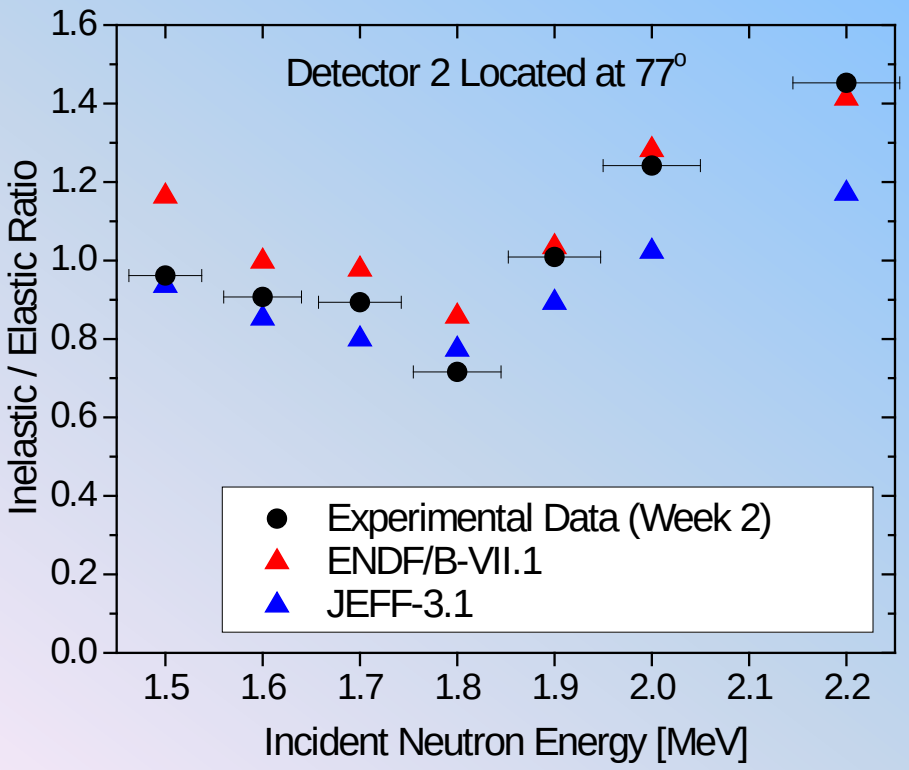
- MCNP was used to calculate the as-measured elastic-to-inelastic neutron ratio for different evaluated nuclear data libraries

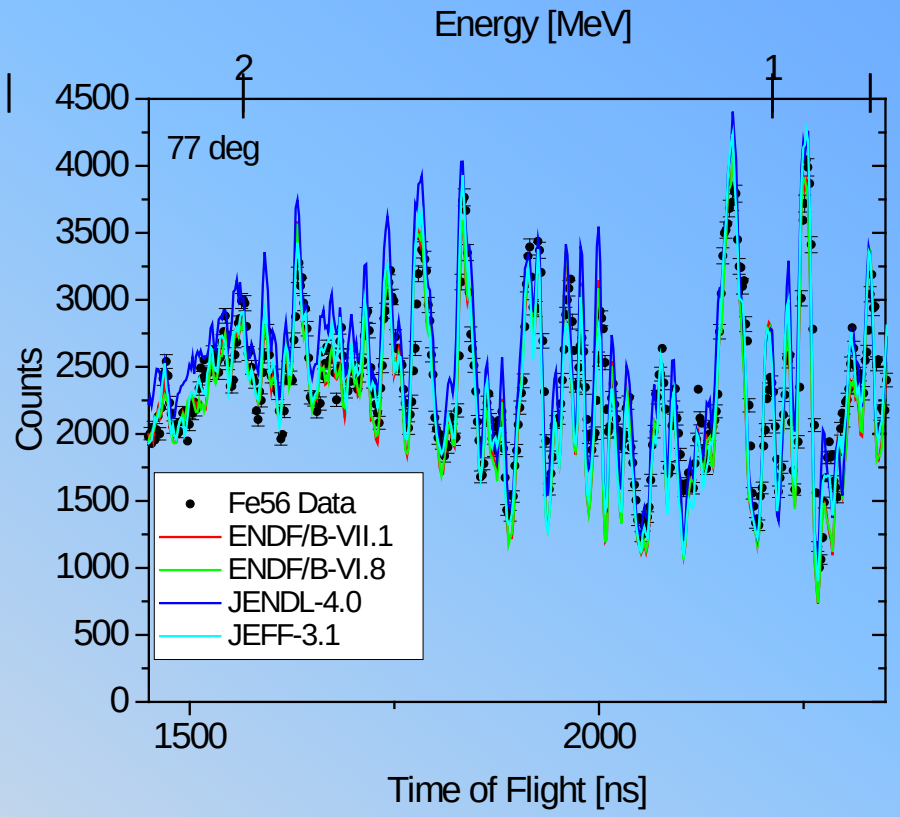




1St Inelastic to Scattering Ratio at 77 deg Experiment and Evaluations

- MCNP was used to calculate the as measured elastic to inelastic neutron ratio for different evaluated nuclear data libraries





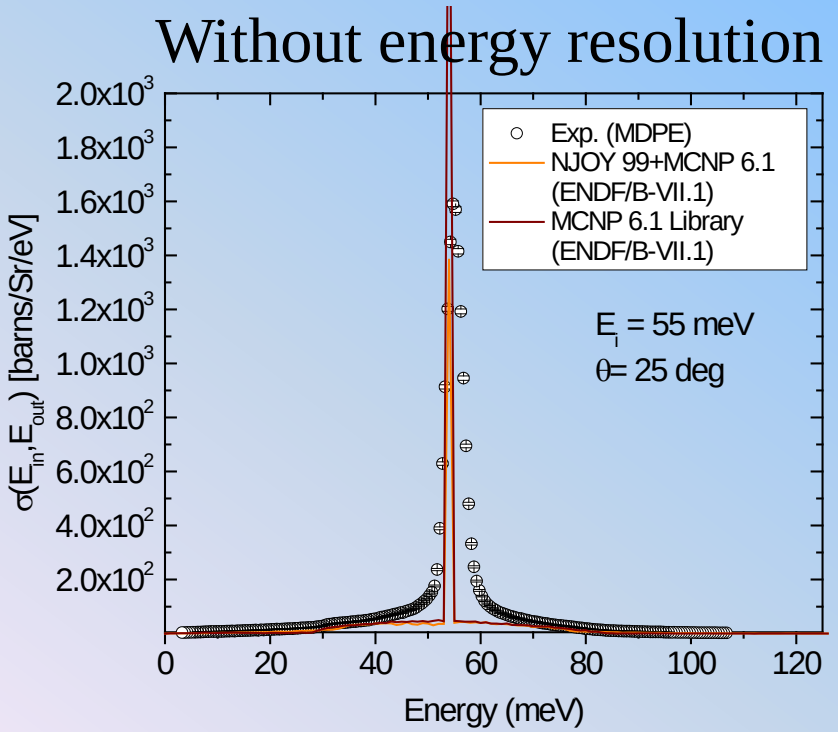
Thermal Scattering Overview

- Analyzed experimental data for water and Medium Density Polyethylene (MDPE) that was measured using SEQUOIA at SNS
- Performed measurements of High Density Polyethylene (HDPE) and Quartz (SiO_2) using the Wide Angular-Range Chopper Spectrometer (ARCS) at SNS at SNS.
  - Quartz measurements were done at 20, 300 550, 600 °C
  - HDPE was measured at 295 K and 5 K.
- LAMMPS code is utilized to calculate the phonon spectrum and scattering kernel for water and HDPE

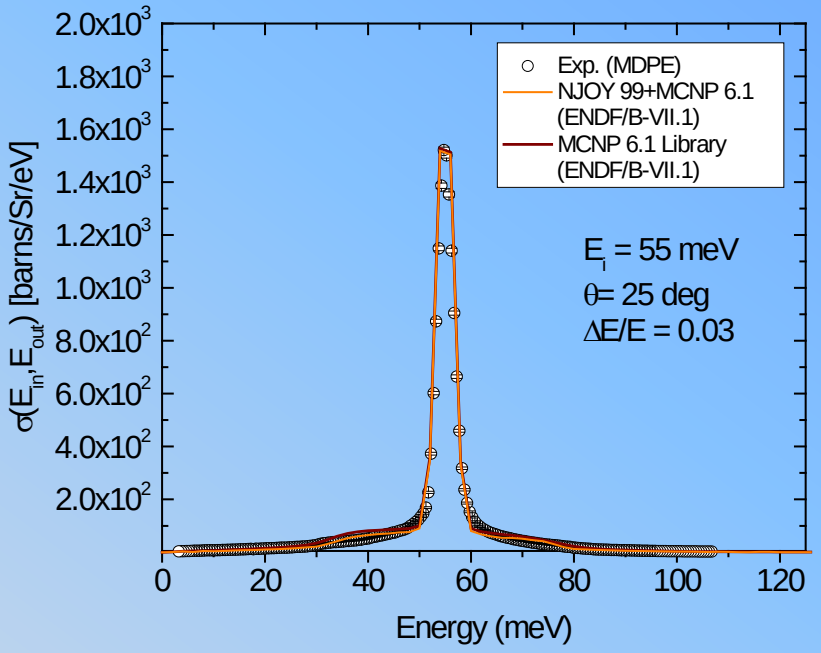
MDPE Data Processing
Spectrometer Energy Resolution

- Use MCNP simulation of the incident energy spread.

Without energy resolution

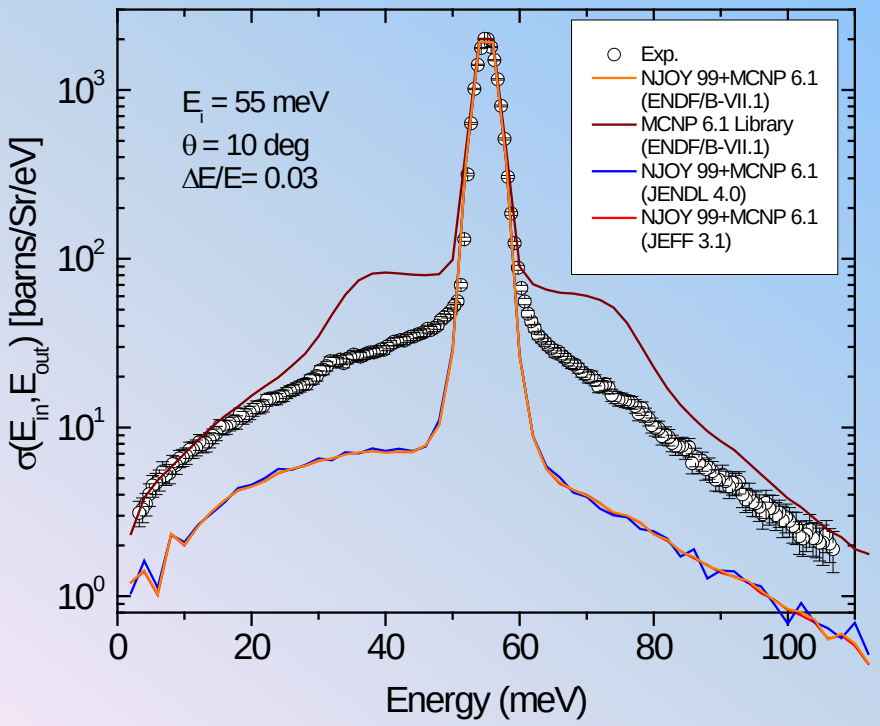


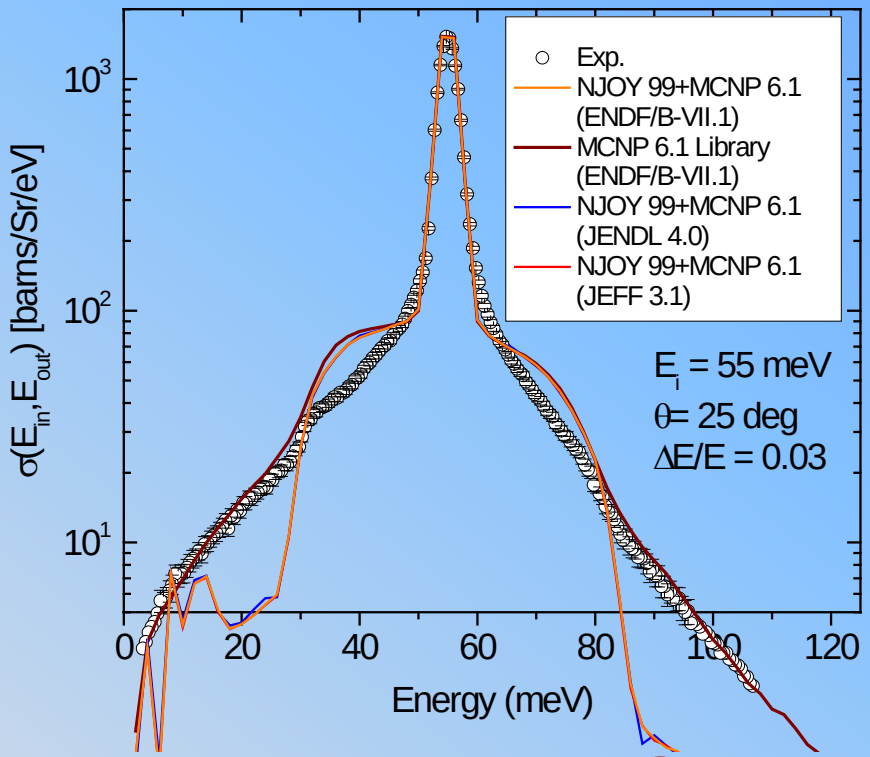
With energy resolution



MDPE Experiment compared with different evaluated data files

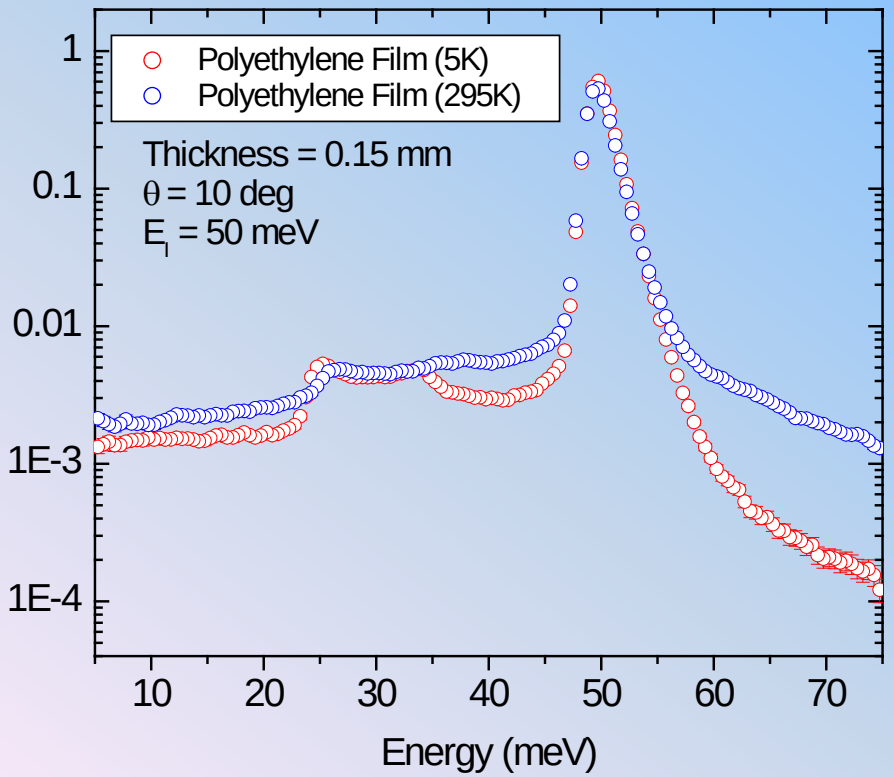
- Comparison with several evaluations
  - More structure and larger differences in forward angles.
  - Possible issues with how we run NJOY/MCNP

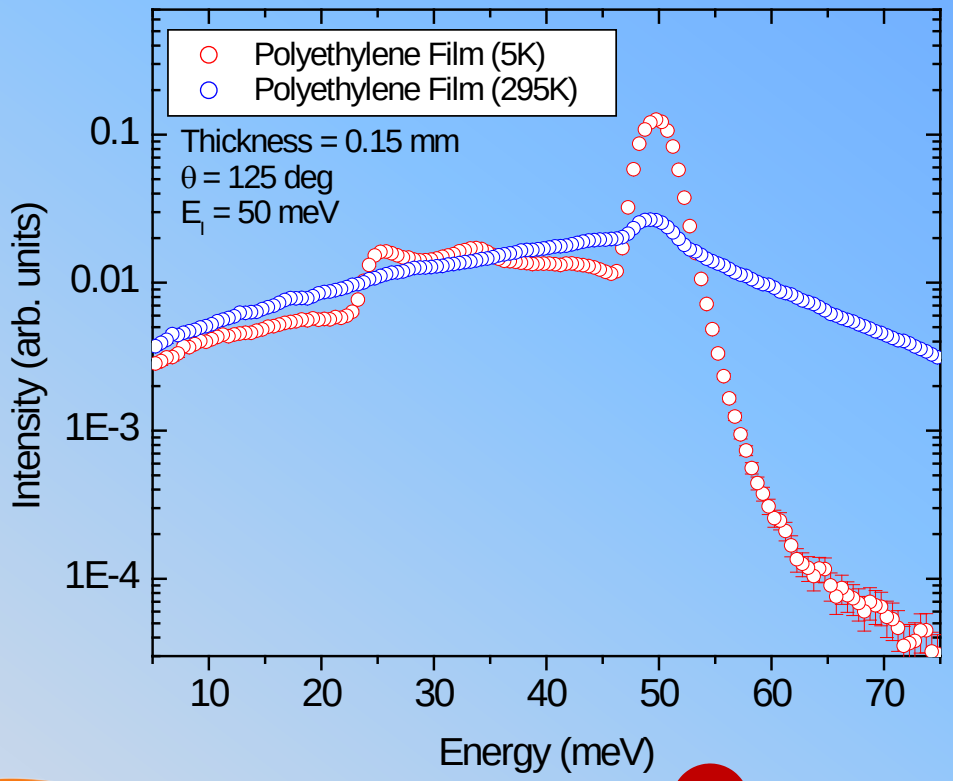




New Raw Experimental Data

- Polyethylene using ARCS-Wide Angle Spectrometer at SNS





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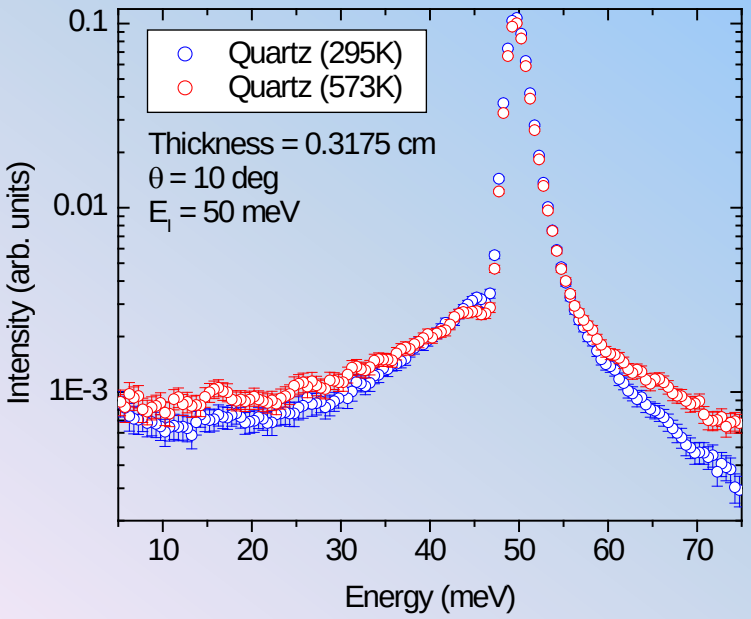
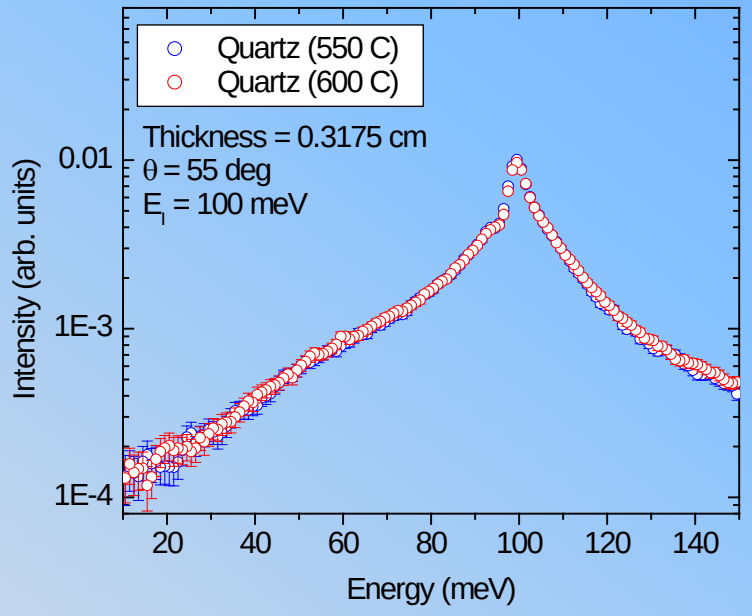
Quartz Crystal

- SiO_2 was measured at multiple thicknesses
  - 0.3175 cm and 0.635 cm (1/8th and 1/4th inches)
  - Temperatures: 20 C, 300 C, 550 C, 600 C



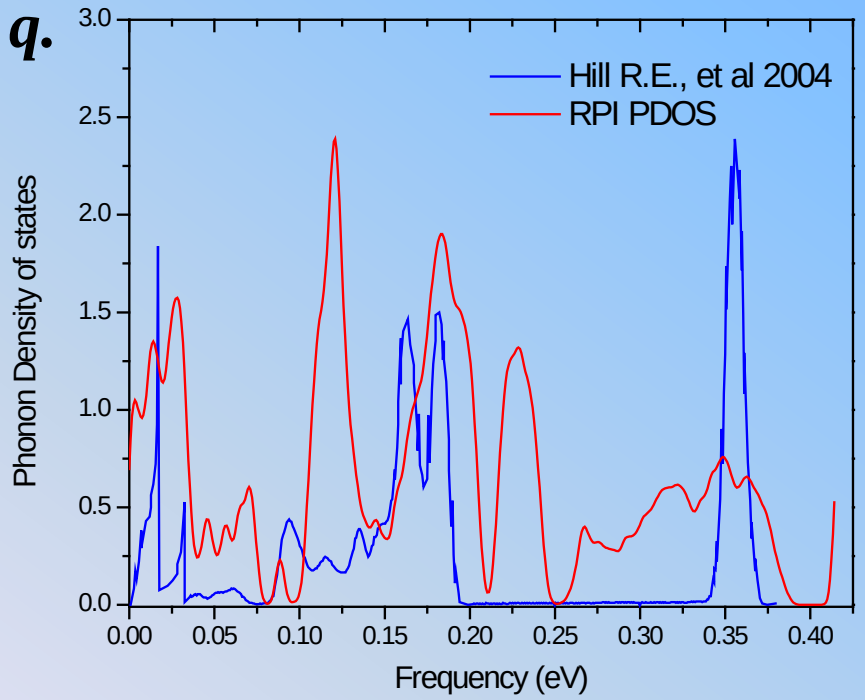


Polyethylene - LAMMPS Simulation

- Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential for systems of carbon and hydrogen atoms.
- Polyethylene (-CH_2-)n chain.
  - 400 molecules in chain, 1200 atoms.
  - 296 K temperature.
  - 0.1 fs (femtoseconds) time step
  - 20,000,000 steps = 2 ns (← This is the time simulated)
- FIX_PHONON
  - calculates the dynamical matrix from MD simulations based on observing the displacement fluctuations.
- Output: binary files containing dynamical matrices whose eigenvalues are exactly the phonon frequencies at wavevector **q**.

Polyethylene – LAMMPS post-analysis

- Post-processing - PHANA code, distributed alongside FIX_PHONON user package.
- PHANA - calculates Phonon Density Of States (PDOS) by evaluating eigenvalues of dynamical matrices at given wavevectors ***q***.



The Scattering Kernel - S(α,β)

- LAMMPS phonon spectrum can be converted to a scattering kernel S(α,β)
- Using incoherent and Gaussian approximation:

$$S(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\beta\hat{t}} e^{-\gamma(\hat{t})d\hat{t}},$$

where $\hat{t}$ is time in units ħ/kT seconds,

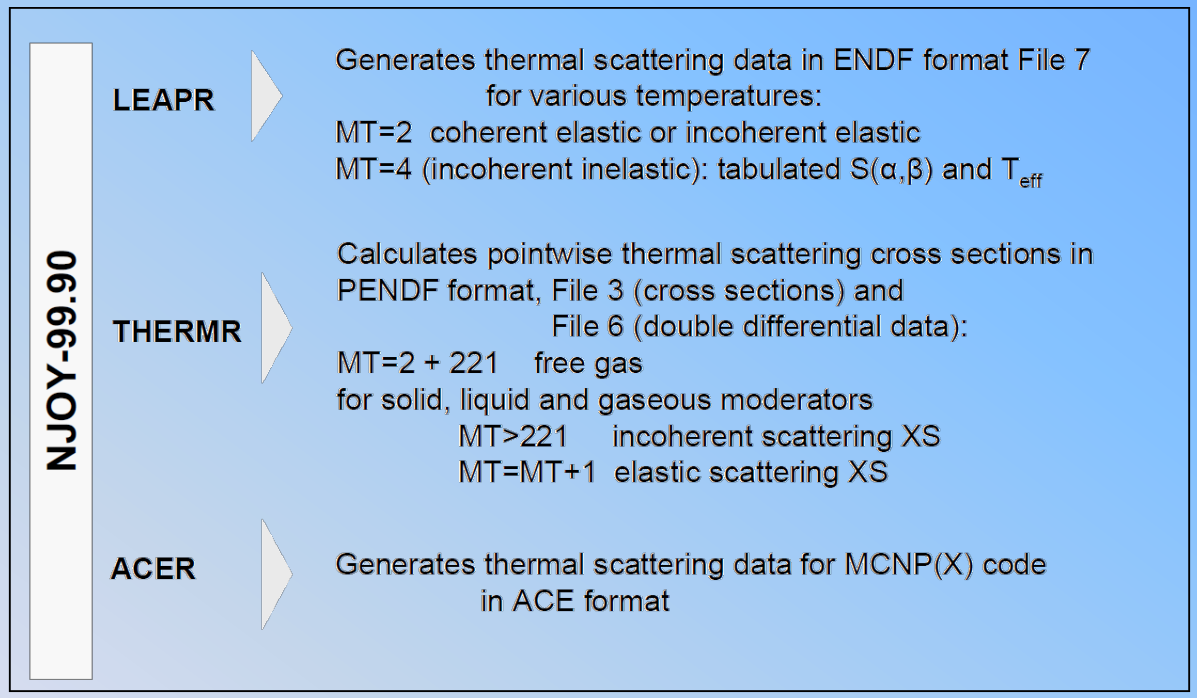
$$\gamma(\hat{t}) = \alpha\int_{-\infty}^{\infty} P(\beta)\left[1-e^{-i\beta\hat{t}}\right]e^{-\beta/2}d\beta,$$

with $$P(\beta) = \frac{\rho(\beta)}{2\beta\sinh(\beta/2)},$$

where ρ(β) is phonon density of states, PDOS.

Polyethylene discussion – S(α,β)

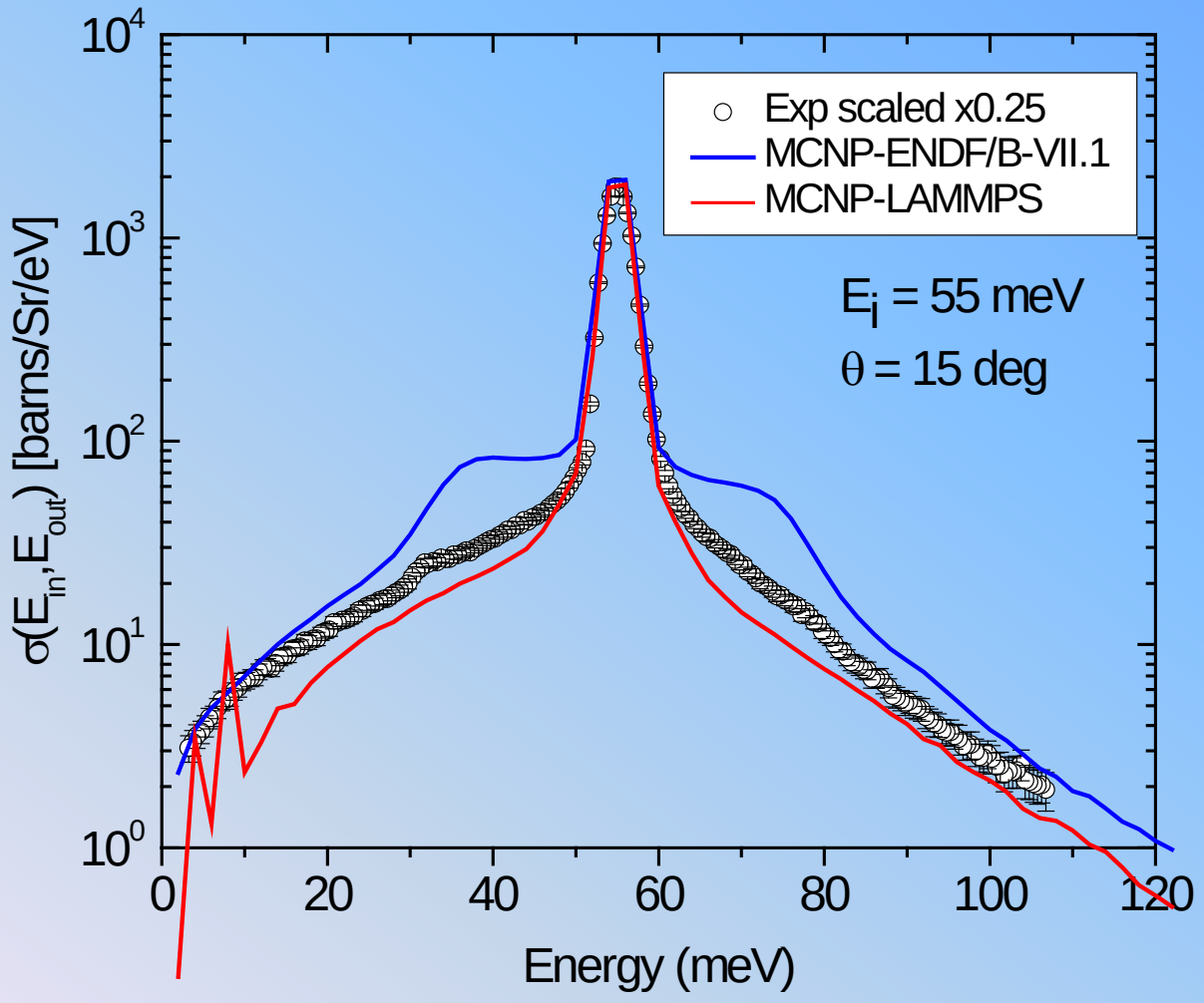
- PDOS →NJOY99 (LEAPR)



- ACE files → MCNP6.1 to generate double differential scattering cross section (DDSCS) to compare with the experiment.

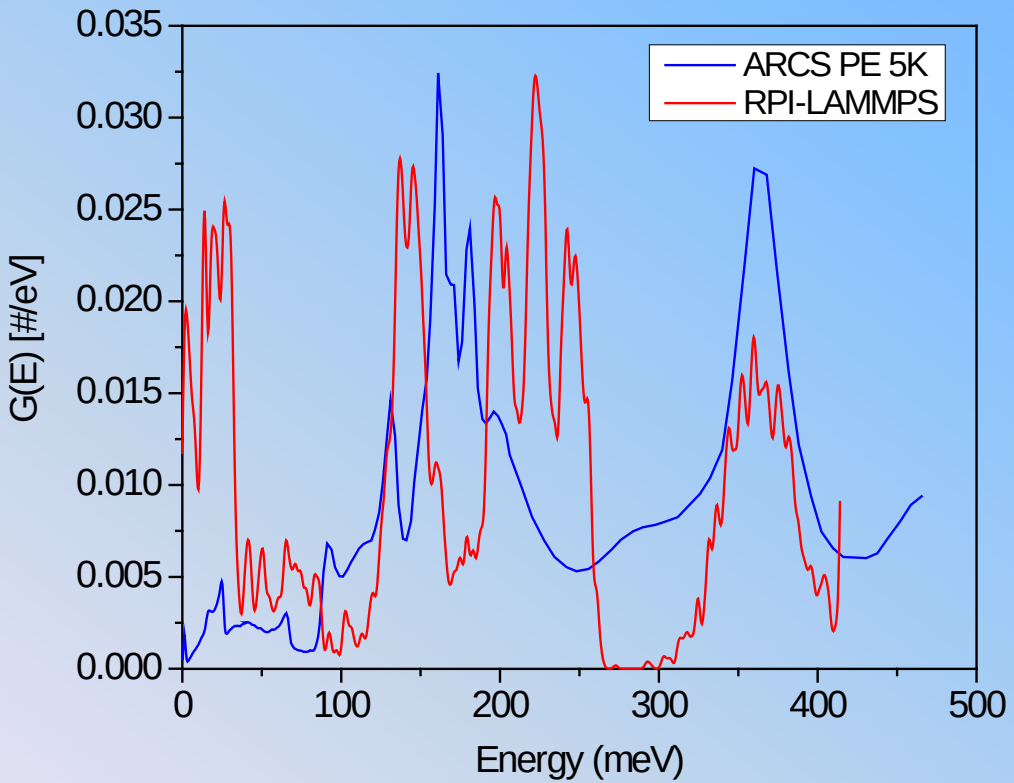
*M. Mattes and J. Keinert, Thermal Neutron Scattering Data for the Moderator Materials H2O, D2O and ZrHx in ENDF-6 Format and as ACE Library for MCNP(X) Codes, IAEA INDC(NDS)-0470, 2005.

Polyethylene DDSCS 15 degrees

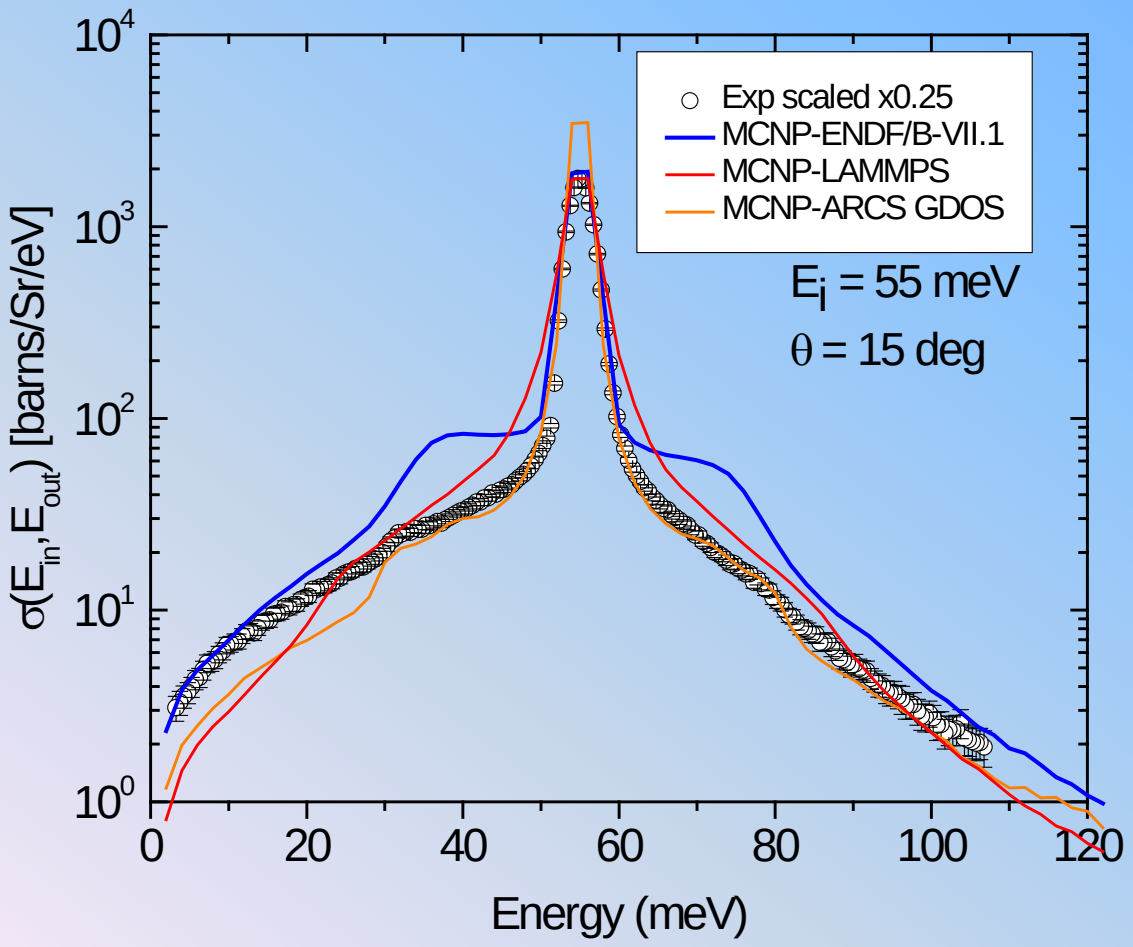


Measured Phonon Spectrum

- Use NIST DAVE code to convert experimental data using one-phonon approximation, to Generalized Density of States G(E) which can be compared with the LAMMPS calculations.
- Some features are similar (at ~150 and ~350) but the agreement is not very good.
- Improved LAMMPS calculations will include a full lattice cell (more than one chain that was now used)



Experimental scattering kernel in MCNP First attempt for HDPE



- As expected the new scattering kernel agrees better with the experimental data
- Need to resolve the elastic peak and the impact of the spectrometer energy resolution.

Future Studies

- Proper identification of the reasons associated with the discrepancies.
- Fit the data with the new experimental data that will be acquired from ARCS at SNS.
- Better understanding of PDOS physics.
- Perform LAMMPS simulations using different force models and try to improve upon the current ones.

LINAC 2020 Refurbishment and Upgrade Plan

- First meeting with SLAC team occurred last week
  - Discussed the requirement and options for the refurbishment project.
- Project timeline acceleration
  - NR/KAPL is staging a significant procurement in FY14.
  - Additional funds will be available in FY15 to complete the purchase of additional klystrons

Recent Accomplishments

- Completed scattering measurements and analysis for ^{56}Fe
  - Show new results for the ratio of the first inelastic state to elastic.
- Developing a new capability to measure capture cross sections in the mid energy (keV) range
  - Detector array was installed
  - Flight path pipes vacuum system was installed.
  - Sample changer was installed.
  - DAQ and analysis software were developed.
  - Resolving problems with two of the detectors.
  - A test of the whole system with sample of B_4C, C, Fe and Mo
  - Planned for another test measurement with Fe.
- Completed measurements of thermal scattering at SNS
  - Quartz measurements were done at 20, 300 550, 600 °C
  - HDPE was measured at 295 K and 5 K.
  - Data analysis and LAMPPS simulations are in progress
- LINAC 2020 refurbishment and upgrade plan in progress
  - First meeting with SLAC group occurred on the week of 3/16/2014
  - Funding schedule accelerated, planning klystrons purchase