Comparisons of simulated and measured ZrH_2 data on SEQUOIA.

NEUTRON SCIENCES

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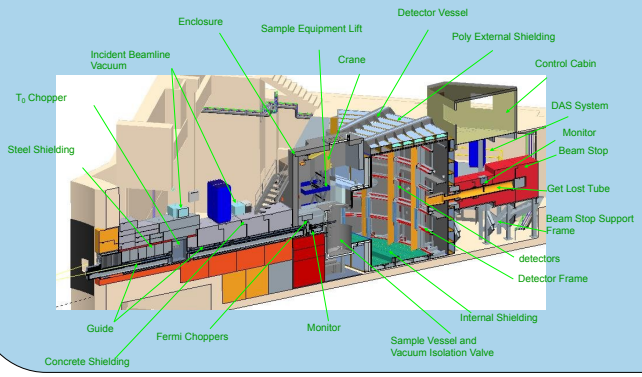
The SEQUOIA spectrometer [1]

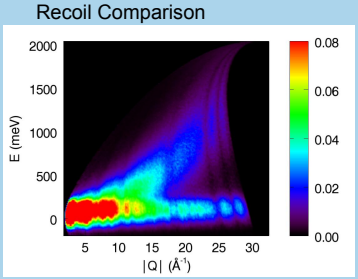


Source	Ambient H20 Moderator	SNS_Source, sct input file
T0 chopper	Vertical axis, 20 cm inconel, narrow bandwidth 10.0 m from moderator	Custom component
Guide	Elliptically tapered from moderator to 0.5 m from sample	Series of Channeled_guide components
Fermi Chopper	3.6mm slits curvatures 1.53 m 600 Hz 18.0 m from moderator	Custom component
Sample	50.0 mm x 50.0mm x 0.1mm ZrH_2 [2] T ~ 8K ;20 m from moderator E_i = 1, 2 eV	Sqw_isotropic[3] with quantum harmonic oscillator or recoil
Detectors	8 packs of 2.5 cm diameter, 1.2m long tubes divided into 128 pixels and placed on a 5.5m radius cylinder covering -30° to -2.5° and 5° to 60° in the horizontal plane and ± 18° in the vertical plane	Three 1.2m tall cylindrical MonitonD components operating in list mode

Details

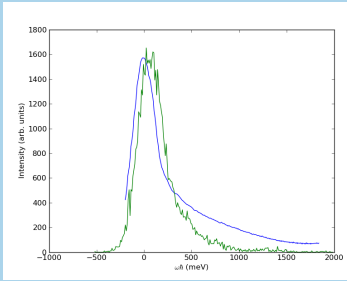
All simulations were performed using the McStas Monte Carlo package [4] for 3e9 iterations. Neutrons that made it to just before the sample were split 10 times to increase efficiency. The simulation data was processed with custom python code. The measured data was analyzed using Dave Mslice[5]

Recoil Comparison



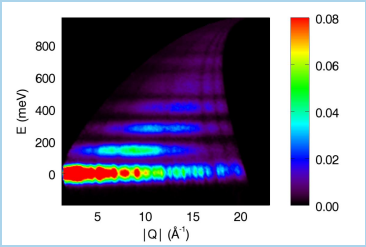
Recoil as measured on SEQUOIA for ~ 2eV neutrons The recoil signal is indicative that the incident neutron energy is greater than the top of the H potential well.

A recoil sqw omega file was used to simulate the scattering.



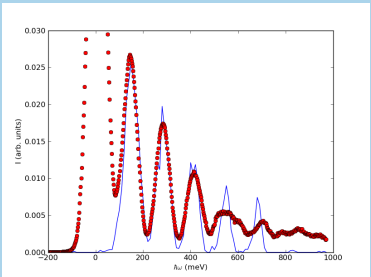
A sum over all Q for both the data (blue curve) and simulation (green curve) An arbitrary scale factor was applied to match the peak heights. Notice the peak shape matches well near the elastic line, significant differences in the large energy transfer tail are still under study. The center offset is due to differences in peak emission time between the simulation and the experiment.

Quantum Harmonic Oscillator Comparison



Quantum harmonic oscillator regime as measured on SEQUOIA for ~ 1eV neutrons Note that 4 phonon peak is quite broad even though the resolution is fine at this energy transfer.

An sqw omega file with peaks in energy and no Q dependence was used to simulate the data. The elastic line was ignored at this point in the simulation process.



A sum over all Q for both the measured (red points) and simulated (blue line). An arbitrary scale factor was applied to the simulation result. There is excellent agreement between the simulated and measured peak shapes for the 1 and 2 phonon peaks. For the 3 phonon peaks and beyond splitting in the lines are observed as in high resolution studies of the 1 phonon peak [6]

Acknowledgements:

We are grateful for discussions with E. Farhi and V. Lynch. T. Sherline and A. Upasani assisted with experiment set up. All work performed at Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 for the U.S. Department of Energy

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