Event Processing Neutron Powder Diffraction Data with Mantid

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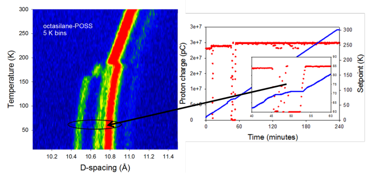
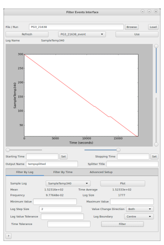
Temperature Ramp with Constant Proton Charge

New measurement mode at SNS allows for setting ramp rate as a function of proton-charge. The advantage is that, for non-kinetic scans, the measurement will adjust for all temperatures to have similar statistics independent of fluctuations in the accelerator energy.



General Event Filtering Interface



Event filtering GUI allows for simple methods of filtering events and log exploration:

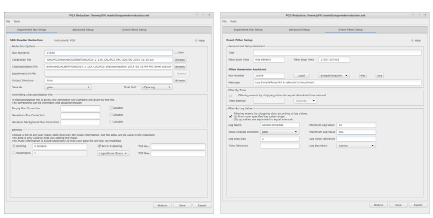
- By log value (threshold and stepping)
- By time steps

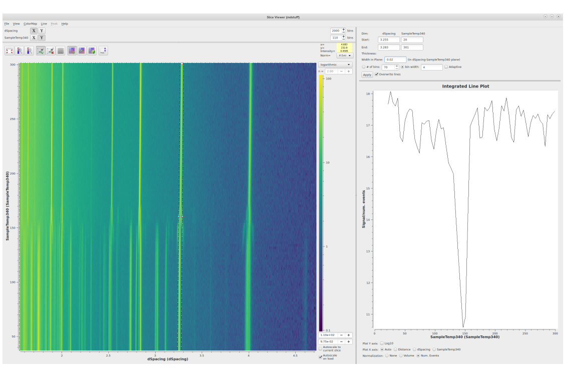
The filtering of events also supports a calculation of when the neutron was at the sample position for comparing to log values.

Rietveld Reduction Interface

GUI provides for common reduction of data for Rietveld analysis. Features include

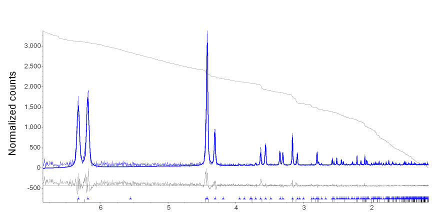
- Support for GSAS, FullProf, and TOPAS file formats
- Common parameters are easily accessible
- Summing files
- Tab dedicated to event filtering





Methyl-ammonium lead chloride

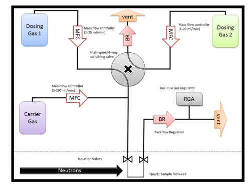
Slice viewer allows for visually exploring parametric data. Arbitrary line cuts through the data can be made and either fitted in the mantidplot application or written to file for use in other software.

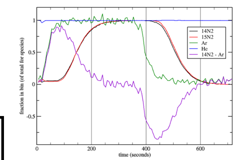


TOPAS fit of 2 effective minutes from 0.25K/minute runs 14 parametric spectra Rwp=12.3

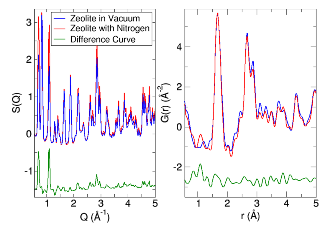
Commissioning a High-precision Gas Flow Cell

High precision mass flow controllers are used to carefully flow dosing gas (0-10 sccm) through a high speed switch, where a carrier gas (0-40 sccm) mixes, and is then piped to the sample. Digital back-pressure regulators maintain the desired pressure at the sample (0-10 psig). Several designs of the quartz sample cell were explored, both a simple U-tube and a tube-within-tube design.





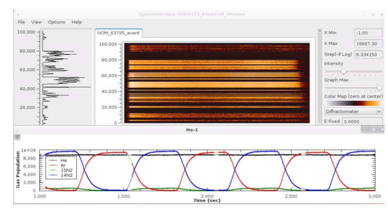
(left) Basic design of high-precision gas flow cell. (above) RGA measured response of Zeolite-X system to Nitrogen/Argon SSITKA measurement performed *in situ* on NOMAD.



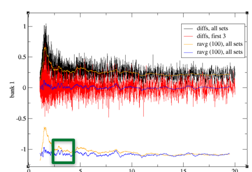
Isotope	Abundance	σ_{coh} (barn)	σ_{inc} (barn)
14N	99.63%	11.03	0.5
15N	0.37%	5.21	0.00005

$^{14}N_2$ and $^{15}N_2$ exhibit a strong difference in coherent scattering lengths. Helium was used as a carrier gas. 3% Argon was mixed in the 14N2 to act as a tracer gas.

Initial analysis shows dramatic change in the structure of the Zeolite in the presence of nitrogen. To examine the differences in between the two N_2 conditions and track time-dependent adsorption behavior, the data must be binned stroboscopically with the Mantid data reduction framework. The differences between the two sample conditions are subtle enough to be pushing the boundaries of available signal sensitivity. The analysis is complicated by the unexpected uptake of water in the samples, as the neutrons prove more sensitive to the introduction of Hydrogen in the system than the N_2 scattering length effects alone.



Stroboscopic rebinning capabilities demonstrated in the Mantid framework



Measured differences in a single bank between sample conditions rebinned stroboscopically. Peaks attributed to nitrogen adsorption have been highlighted.

For the first time, steady state isotopic transient kinetic analysis (SSITKA) of catalytic materials can be performed while simultaneous neutron PDF data is measured. In this way, the data can be stroboscopically rebinned using the Mantid framework to study kinetic processes occurring at timescales too short for conventional neutron PDF analysis. This work represents the combined efforts of the Spallation Neutron Source, the Center for Nanophase Materials Sciences, and Colorado State University.

Future Development

- Support for user created event filters
- Providing additional information to modeling packages (e.g. GSAS, FullProf, TOPAS, PDFgui, RMCProfile)
- Tools for detecting phase changes and determining consistency in data

There is a challenge for modeling packages to improve support for parametric studies as the parameters will vary with more values

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