HYSPEC Status, February 5, 2013

On June 22, 2012, we provided a status report on the HYSPEC instrument; this is a quick follow-up report on each of these issues.

1. User program for unpolarized neutrons

   On November 7, 2012, we went through an internal, operational, instrument readiness review for unpolarized neutrons for users. The report will be signed soon, and most action items are already completed. We are about to begin preparing for the extended commissioning plan report, which demonstrates science readiness, and for which we will be asking for feedback from the IDT Executive Committee.

   In the last call for proposals, ORNL received 12 requests for beamtime through the user program. Of these, four successfully went through the Science Review Committee (SRC), and the others were diverted to instrument development proposals. These were changed because the techniques and/or sample environments to be used in those experiments have not yet been demonstrated on HYSPEC.

   Our four priorities this cycle are: satisfy the NSCD criteria for being a user instrument for unpolarized neutrons, host those user experiments that were approved by the SRC, continue polarization analysis commissioning, and prepare for and host those experiments that were changed to instrument development proposals.

   We expect to hire a new instrument scientist this spring, to join the HYSPEC instrument team in its commissioning and user-program activities.

   The next call for proposals will continue to show HYSPEC as having only partial availability, so that we can continue our commissioning with polarization analysis.

2. Polarization commissioning

   Previous status:
   The Heusler focusing array was found to have a flipping ratio of about 25 between 7.5 meV and 50 meV for the unfocused beam. The Helmholtz-like coil support was reinforced and coated with boron nitride. Offline tests and modifications for the Mezei flipper were made. We received a design from PSI for a magnetizer, and resumed discussions for transfer of the polarizing supermirror array to the US.

   Update:
   From Aug 24 to Aug 27, we used two polarized 3He cells (‘Trojan’ and ‘Chang’) in the black solenoid (same setup as in the spring) to measure the flipping ratio of the Heusler crystal at HYSPEC, but this

time with the vertically focused neutron beam. ‘Trojan’ has a pressure of 1.3 bar, a diameter of 6.9 cm and a thickness of 11.9 cm, initial 3He polarization of 35% and a lifetime in the solenoid of 80 hr. ‘Chang’ has a pressure of 2 bar, diameter 12.1 cm and thickness 10.7 cm, initial 3He polarization of 65% and a lifetime in the solenoid of 40 hr. The 3He polarization was flipped with Adiabatic Fast Passage (AFP) NMR for flipping ratio measurements of the entire system, and ratios measured for the full system ranged from 16.75 at 7.5 meV to 3.13 at 90 meV. However, we had slightly different aperture configurations for with-cell vs. without-cell, and therefore obtained inconsistent results concerning Heusler polarization.

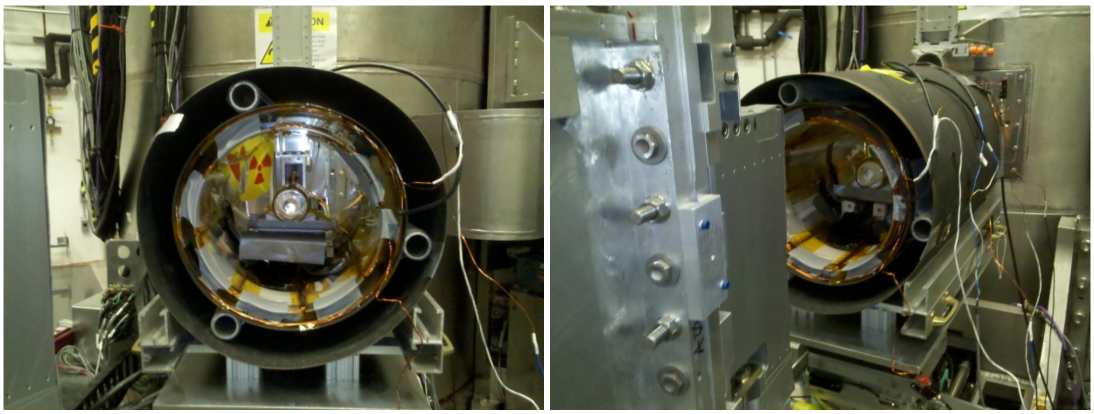
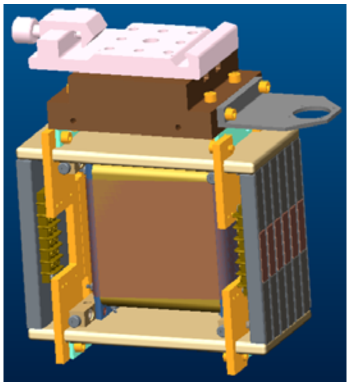


Figure: ‘Chang’ cylindrical cell in solenoid for initial focused beam polarization tests.

We mounted, aligned and performed offline 3He lifetime tests with the Helmholtz-like coil on the detector vessel. We found a lifetime of ~ 100 hrs for the cell ‘Chang’ that was not significantly reduced by the addition of CCR-19 at the sample position. However, changing from a weak optic rail-mounted guide field to a much stronger one showed great impact on the cell lifetime (100 hrs to 25 hrs).

Roger Pynn, Bill Hamilton and Steven Parnell took our Mezei flipper to CG1 at HFIR for initial characterization with neutrons. It was found that anodized aluminum strip-wire performed better than the bare aluminum wire we had first used, most likely due to local fields between windings depolarizing the neutron beam. They achieved a system flipping ratio, using the Mezei flipper, of ~10 at 5 meV. Using lessons learned from this experiment and later work at HYSPEC, we have designed an improved Mezei flipper, and are about to begin fabrication.

 Figure: Mezei flipper redesign.

At HYSPEC, we performed neutron polarization and transmission measurements at several Ei's and cylindrical cells of various sizes and pressures. We found that the neutron monitor in the beam did not affect neutron polarization. Our first attempt produced ambiguous results, but with lessons learned we concentrated on the use of a large-diameter cell, and careful preparation of apertures about the 3He cell. We used Cadmium sheet upstream and downstream of the cell, and boron nitride plates to the sides to shield against the RF flipping coils. For direct beam measurements, we also employed a cadmium pinhole at the sample position.

Later, we operated at 15 meV using the Helmholtz-like coil and the 'Chang' cylindrical 3He cell at 2 bar. We were able to flip the neutrons upstream of the sample position using the Mezei flipper and change polarization analysis using RF. We performed measurements in the direct beam, using a cadmium pinhole at sample position. Initial 3-He polarization was about 60% and the lifetime was 76 +/- 16 hr. We measured flipping ratios via flipping the 3He polarization at the start and end of this 3-day run, as well as measuring unpolarized transmission. With measured system ratios of 14.7 and 7.3, respectively, we derived a Heusler array flipping ratio of between 19.3 and 25. The main uncertainty comes from the lifetime measurement. The system ratio at the start of this run using the Mezei flipper was 9.2.

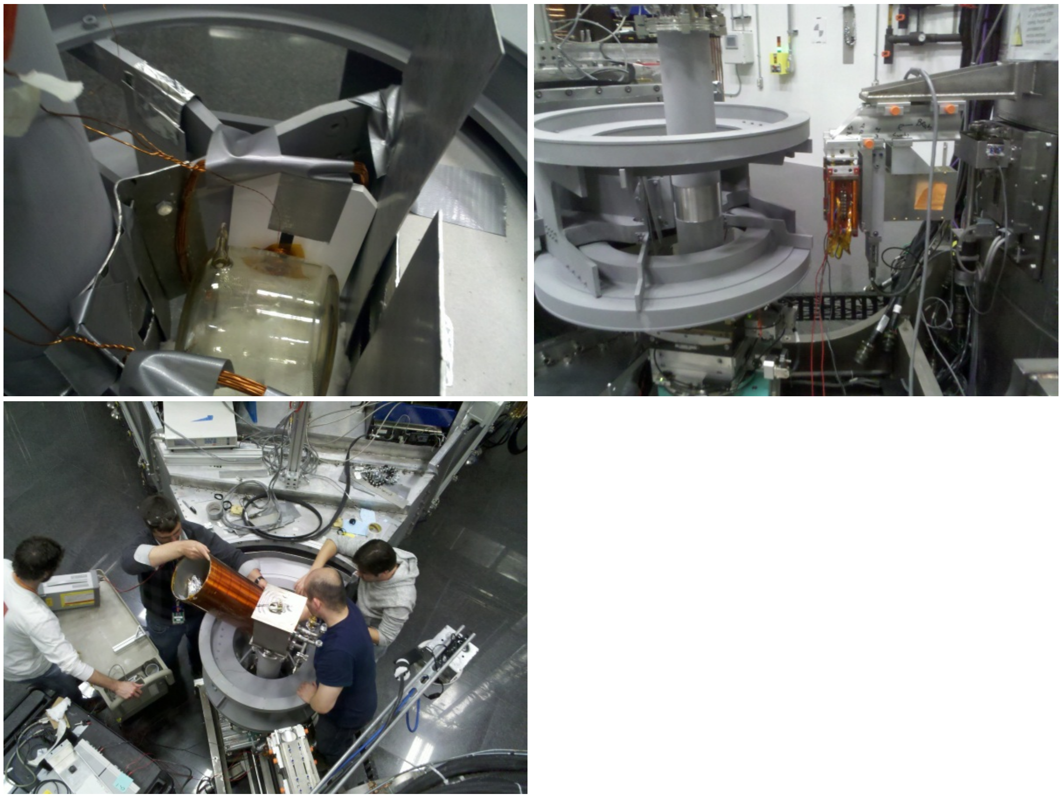


Figure: December setup with ‘Chang’ cylindrical 3He cell. Shown inserting the cell are Peter Jiang, Steven Parnell, Dan Brown and Hunter Culbertson. Final order of optic rail components after optimization is shown at top right, and includes a guide field assembly, neutron monitor, fixed aperture and Mezei flipper.

In between these direct beam measurements, we observed a ratio of 0.68 in spin-flip vs. no-spin-flip scattering from Vanadium at 15 meV, using the Mezei flipper to change the polarization of the incident beam. Since these measurements were taken 25 hours after initial He-3 polarization measurements, the 3-He polarization was roughly 43%. With the 2 bar pressure in the ‘Chang’ cell, transmission was low, so each of the two measurements lasted 1.8 hours. Masking in reduction was chosen to avoid a powder diffraction line, and time binning was chosen to avoid the prompt pulse background feature. The expected ratio in scattering measurements is 0.5 for a perfectly polarized system and only incoherent scattering from vanadium, but factoring in polarization efficiencies of the Heusler focusing array, Mezei flipper and 3-He cell, we expect a ratio of 0.60. Therefore, our measured ratio of 0.68 is within ~13% of our expected ratio.

We also used a Heusler single crystal in yoke as an independent analyzer for additional characterization and Mezei flipper tuning. This crystal was mounted at sample position, with the Helmholtz-like coils running, and no 3He cell was used for subsequent analysis. A system flipping ratio of 9.9 was found for Ei = 5, 20 and 50 meV, using the Mezei flipper to change polarization.


Figure: Heusler single crystal in yoke, mounted at sample position.

For the 3He gas transfer system, the new titanium syringe bellows is in fabrication, and the new cart and valve have complete designs and are about to go out for procurement.

We have prepared two compact sets of optic-rail mounted apertures to use in place of our variable apertures, when performing polarization analysis measurements. This gives us the space to use our optic-rail guide fields and Mezei flipper, and provides a narrow gap between guide field components which helps to preserve neutron polarization from the drum shield to the sample. A set of interchangeable fixed-width and fixed-height boron nitride plates define the apertures.

Discussion with our PSI colleagues continues, for the shipment of the polarizing supermirror array to the US. We are developing a simpler design for the magnetizer that will be much less expensive to build than the one prepared from existing coils at PSI. We are also designing a simple vertical guide field system to maintain polarization about the sample and to the polarizing supermirror array.

3. New data acquisition system prototyping

Beginning in June 2012, HYSPEC became the prototype instrument for implementing a new event-based data acquisition system, that broadcasts the streaming data to both an event translation service (speeding translation significantly) and a live-viewing mode in the Mantid data analysis program which permits viewing in Q-E space. We are leveraging the computing power and expertise at ORNL, by teaming with ORNL's Computing and Computational Sciences Directorate in development, and by a parallel file system for storage of the new data files. We also have the option to use a parallel computing platform for some Mantid operations.

For an overview of this developing system, please go to the following news link:
http://www.hpcwire.com/hpcwire/2012-12-04/neutron_science_and_supercomputing_come_together_at_oak_ridge_national_lab.html

This system is functioning and being further developed, in parallel with the operation of the legacy data acquisition system at HYSPEC. This strategy has allowed the HYSPEC team to continue commissioning, relatively undisturbed by developments in the new system. It has also allowed the new development team to refine their system without the pressure to patch-repair problems to resume operation.

4. Prompt Pulse Background

Previous status:
A time dependency to the prompt-pulse feature was found to be caused by the opening of the BL 13 secondary shutter. A facility wide shutter test determined that the bulk of the background remains when all shutters are closed. Gradual time variations in the background feature remained unexplained.

Update:
Since an attempt at shielding, using a 4-high, 3-wide stack of temporary blocks at the boundary between BL 13 and BL 14, did not affect HYSPEC's background, and we can only go one level (~0.6 m) higher, we have not pursued additional shielding strategy/tests to mitigate the BL 13 secondary shutter.

The portable detector array was disassembled for use elsewhere at ORNL. We know of a possible hot-spot atop BL-18 near the monolith, but have not attempted a shielding test there yet.

An automated reduction routine has been prepared, that accounts for the prompt pulse when selecting a time-independent background range. This automated reduction routine uses the Mantid analysis program to generate SPE files that can be read by other analysis programs like MSLICE and HORACE.

5. Other background

Previous Status:
Scatter from air, the drum shield, optics upstream of the sample, sample environments, and the detector vessel have been minimized using a crude prototype shield about the sample. Based on lessons learned from making this prototype, and using feedback from both ORNL staff and friendly initial users, we began coordinating with engineering support to develop a more permanent shielding solution.

Update:

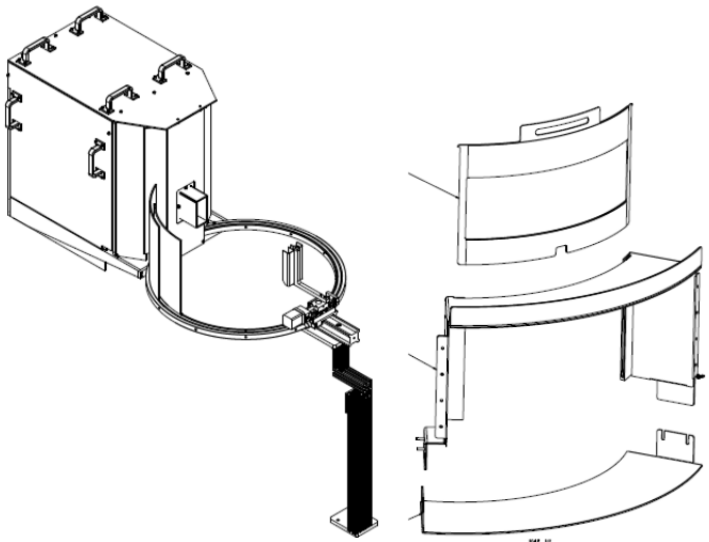


Figure: Engineered design for components surrounding radial collimator and optic rail components, and new beamstop.

The design has been completed and fabrication begun. Shielding assumes a 1.8 m distance between focus element and sample, and works with our orange cryostat and our newly arrived large-diameter CCR tails. A new beam stop will function with both high and low detector vessel angles.

6. Detector vessel location, motion and collision avoidance

Previous status:
Scannable control on the control PC was implemented.

Update:
Drum shield and detector vessel motion have been reliable since October 2012. A script for automating the setting of the incident energy has been developed and tested.

Early in the fall 2012 cycle, we experienced mechanical problems with both the detector vessel stage (worm gear bent) and the drum shield rotation stage (keyway engagement problem). Using the worm gear from the spare detector stage and a new keyway for the drum shield motor/gear engagement, we were able to repair both problems.

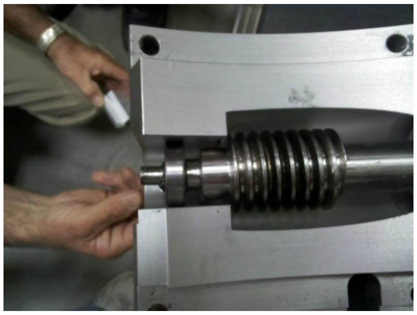


Figure: Worm gear and housing. Worm gear was replaced.

To minimize the chance of future worm gear damage, we have modified our worm-rotation encoder system and limited motion on both systems to a maximum of 1 degree per 10 seconds. We also now have in hand 4 spare worm gears.

Because the drum shield stage encoder is on the motor shaft, we temporarily lost position of the drum shield. Position was regained with help from survey and alignment. We have designed, and will soon install, an encoder for the pinion (a more direct measure of drum shield angle), and an angle indicator at the bottom of the drum shield, to more easily recover in the future.

We have also revisited our limit-switch logic, to minimize the chance for sudden stops. The 'flapping ears' that straddle the entrance window of the detector vessel, were never commissioned and we have found we don't need them. We also no longer need the beam stop that was mounted to an elevator just downstream of the sample, because our new beam stop system will work with the detector vessel at shallow angles. To prevent the collision of the detector vessel with the former beam stop on elevator, and to open and close the flapping ears, we had been stopping the detector vessel rotation stage at angles of +/- 70 deg, causing significant deceleration and stress on that rotation stage. However, we have now removed that logic from our motion control system. We continue to re-evaluate the rest of the limit switch logic that concern the proximity sensors and swinging arm limit switches.

Experience with the proximity sensor system caused us to recognize blind spots at the back corners as likely collision points with walls or cart-equipment. New sensors on the detector vessel, and/or light curtains on the walls, are currently planned to reduce the chance of collision further.

7. Recent activity with sample environments

Previous status:
CCR-19 had become our workhorse sample environment, with support equipment on the drum shield to aid in cable management. Larger OVC's were almost ready for procurement for the CCR's.

Update:
The new OVC's and larger diameter heat shields for the CCR's have arrived, and the one for CCR-19 has been used for several experiments. Background observed earlier has been reduced. Experience

with user sample supports has motivated the fabrication of a flexible set of adaptors and spacers.

The dedicated orange cryostat has been retrofitted with those components our sample environment support prefers. Most offline testing by our sample environment group is complete. A new tail just arrived, to allow for safer tilting.

CCR-10 has been fitted with a sapphire switch and has been used as a high temperature CCR, with a temperature range of 10 to 450 K. Work has begun to dedicate that sapphire switch to CCR-10.

Now that the shield blocks behind the rolling door have been removed, we are planning to demonstrate the transfer of SLIM SAM through that door later this spring in preparation for some 5 T experiments.

8. Recent activity, general performance

Previous status: the coarse collimator inside the detector vessel was removed.
Update: we suspect that we observed scattering of the incident beam from the coarse collimator mount so have now shielded that mount.

Previous status: radiological studies were begun to determine whether the stacked shielding behind the rolling door was truly required.
Update: radiological studies are complete and we have removed the stacked shielding behind the rolling door. This will enable more efficient transfer of larger sample environments through the rolling door.

Previous status: we refined our formula for setting the Fermi chopper phase for a given Ei.
Update: Using the refined formula for Fermi chopper phase, and the ability to move the drum shield from the control computer, we have prepared a PyDAS command line and scriptable routine to set both incident energy Ei and Fermi chopper frequency. With this, we have performed overnight sets of runs with Vanadium, varying both Ei and frequency. Preliminary reduction suggests that our elastic peak is centered at zero energy transfer.

Previous status: we were beta-testing new electronics and software that are to be implemented at instruments throughout the SNS.
Update: the FEM 10 and timing boards continue to work well and are being installed at other instruments.

Previous status: the major leak that was found to be under the downstream chopper racks was left alone, due to expected 2 month downtime and continuous work. Disk choppers were tested and found to function up to higher pressure. Pressure dropped in the springtime to ~70 mTorr.
Update: pressure remained low through the summer, then in October began rising again gradually. There were no pressure spikes during this past year, so we suspect there are no new major leaks.

Current pressure is ~250 mTorr, but this is acceptable for running the T1A chopper and for neutron transmission. We will continue to monitor the pressure, but based on last years' experience we expect the pressure to fall later this spring. We are prepared to fabricate windows to isolate the T1A chopper, if required after a new major leak forms.

New: we are preparing a set of planning tools to enable users to better plan their experiments. These include resolution and flux plots, configuration safety checks (whether the detector vessel will hit a wall), and the beginnings of crystal planning tools (finding Bragg peaks, TobyPlots, etc.). These tools can be run from a python command line, and there are versions (soon to be re-merged) that work with both the Analysis cluster and on PYDAS. We are still testing and debugging these routines.

New: On our secondary shutter, one of the limit switches began to catch, so it was replaced. When repairing this limit switch, we also removed neutron monitor 1 from the beam; this white-beam monitor was useful for initial commissioning, but has been ignored since, and contributed 4 mm of Aluminum to the incident neutron beam path. We have fabricated brackets to prevent this from happening in the future, and will install those at an upcoming outage time.

New: Data files are being automatically reduced to *.nxspe files, for immediate use in Dave's mslice. These reduced files do not yet account for detector efficiency or empty can background, but do provide a convenient way to understand the data and decide what to do during experiments.

New: We have designed and built a laser alignment tool that mounts on the optic rail upstream of the sample.

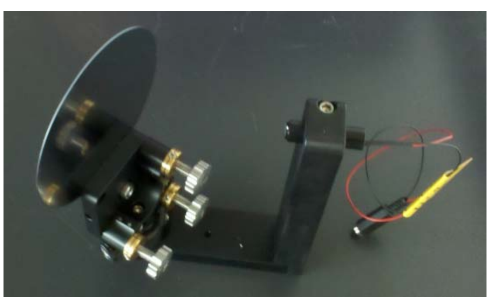


Figure: New optic rail-mounted laser alignment tool

New: We have successfully demonstrated a technique for data acquisition that was pioneered by the ARCS instrument team, and is now an optional mode at both ARCS and CNCS. During a single run, the sample is slowly rotated continuously back and forth, in a desired angle range. For reduction, Andrei Savici has prepared a routine using Mantid that exploits the event data format, by grouping detector events by sample angle into separate *.nxspe files. Two recent users (I. Zaliznyak and J. Wagman) have acquired their data at HYSPEC in this way.

9. Visiting scientist from ANSTO

We had the opportunity to collaborate with Dehong Yu for a month this past fall, and he will return for a month in the spring. Dr. Yu is the instrument scientist for Pelican at ANSTO, an instrument similar in design and goals to HYSPEC. During his visit we did much of the polarization analysis commissioning work for this past fall, and hosted Dr. Greven's team on an experiment.

10. Recent activity with users

Hagen/Shapiro: Cuprite (IPTS-8072, Aug 27-29):

A single crystal of the negative expansion material cuprite (Cu_2O)was studied previously on 3-axis instruments at Munich's PUMA, NCNR's BT7 and HFIR's HB3. When measuring LA phonons along the [00ζ], [ζζ 0] and [ζζζ] directions, we observed additional intensities which qualitatively agree with the TA phonon dispersion, and should not be present. These additional features were observed from zone center out to the zone boundary along [00ζ], out to ζ =0.4 along [ζζ 0] and out to ζ =0.3 along [ζζζ] are not due to resolution effects. Our goal at HYSPEC was to generate a map of Q and E in order to compare TA phonons to the anomalous scattered intensity in the LA directions, away from symmetric directions.

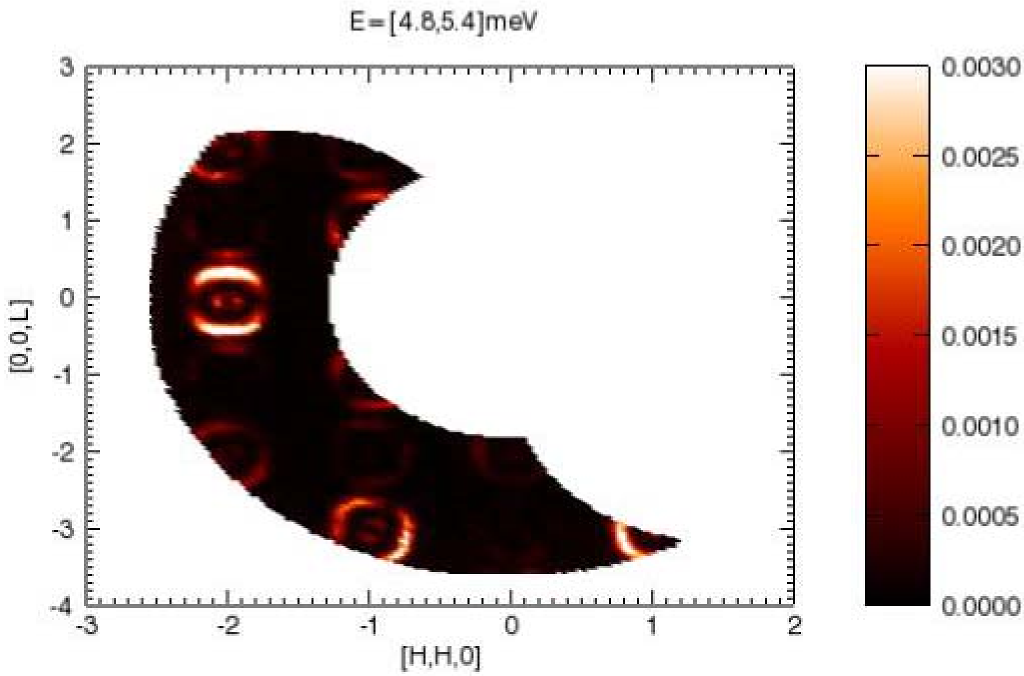


Figure: An 0.6 meV thick slice at E=5.1 meV, in the HK0 plane. Here, we qualitatively confirm that the TA phonons have the same scattered intensity for all directions except for along the LA directions, where the intensity is reduced. The LA phonons are visible inside the TA phonons about (-1,-1,-3) and (-2,-2,0).

The cuprite sample was being studied during the demonstration of live data streaming in Mantid. Please see the following link to see how that data was acquired:
http://www.youtube.com/watch?v=iGAIWoPMbL4&feature=em-share_video_user

M. Stone (IPTS-8137, Aug 31-Sep 4):

Matt Stone has been measuring the same powder sample of CrCl2 at HYSPEC and the other direct geometry spectrometers at the SNS, to compare the relative performance of these instruments.

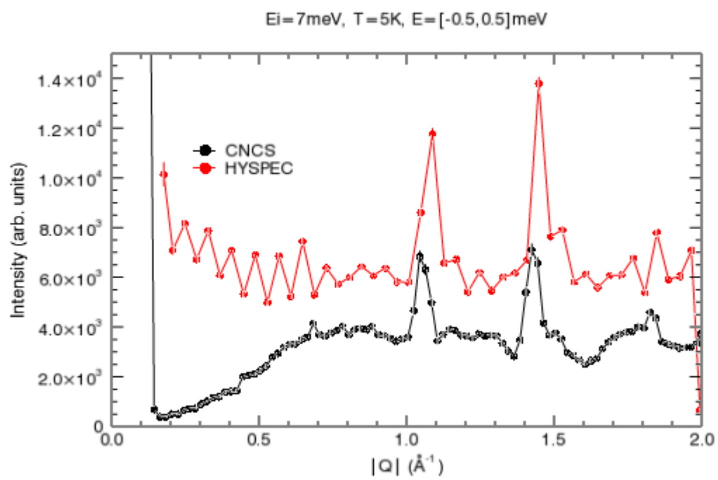


Figure. Intensity as a function of wave-vector transfer for CNCS and HYSPEC integrated between -0.5 and 0.5 meV energy transfer.

Delaire & Chen (IPTS-8132, Sep 7-12):

$KTaO_3$ is a well-known incipient ferroelectric material (quantum paraelectric), exhibiting anomalous phonon dispersions[1,2]. By alloying with $KNbO_3$, a high temperature ferroelectric, the Curie temperature and associated structural phase transitions can be controlled. We have observed anomalous thermal conductivity behavior above the Curie temperature in insulating $KTa_{1-x}Nb_xO_3$ crystals, likely related to the soft phonon mode associated with the ferroelectric instability[3]. In addition, strong electron-phonon interactions are suggested by the significant suppression of the thermal conductivity in semiconducting, Ca-doped materials[3]. We have selected to use inelastic neutron scattering to probe the structure and phonons in single crystals to gain insight into the crystallographic instabilities and thermal properties of these materials

In this first experiment on Hyspec, we have measured phonons in $KTa_{1-x}Nb_xO_3$ crystals as a function of temperature, in order to investigate the behavior of the soft transverse-optic mode. Measurements were conducted on a large (mass=15.2g) single-crystal of nominal composition $KTa_{1-x}Nb_xO_3$, x=0.12. The sample was aligned with (h,k,0) as scattering plane, and mounted inside a displex. The detector bank was placed at high scattering angles (center angle =70deg), to maximize the phonon scattering intensity. Measurements were performed both with and without vertical collimation. We used Ei=25meV, chopper at 420Hz. Data were collected on range of orientations of the crystal in order to map the phonon dispersions, focusing on the transverse optic and acoustic branches along [0,k,0], in the Brillouin zone (200). We measured a range of ~100degrees with 1deg steps. Measurements were performed at T=300K, and T=120K (the range of angles was more limited at low temperature).

Figures below show data for the scattering intensity S(**Q**,E) at 300 and 120K, respectively. The TA and TO branches are clearly identified, and the soft nature of the TO mode at the (200) zone center is also observed. In addition, the TO branch further softens upon cooling, with a minimum TO phonon E<5meV. This corresponds to a nearly ferroelectric behavior. The Curie temperature for the ferroelectric transition in this crystal is estimated T~80K. We plan to measure the behavior of the TO branch across the ferroelectric transition in further experiments.

---

[1] J.D. Axe, J. Harada, G. Shirane, Phys. Rev. B **1**, 1227 (1970).
[2] E. Farhi, A.K. Tagantsev, R. Currat, B. Hehlen, E. Courtens, and L.A. Boatner, Eur. Phys. J. B **15**, 615 (2000).
[3] W. Siemons, M.A. McGuire, V.R. Cooper, M.D. Biegalski, I.N. Ivanov, G.E. Jellison, L.A. Boatner, B.C. Sales, and H.M. Christen, "Dielectric-constant-enhanced Hall mobility in complex oxides", *submitted.*

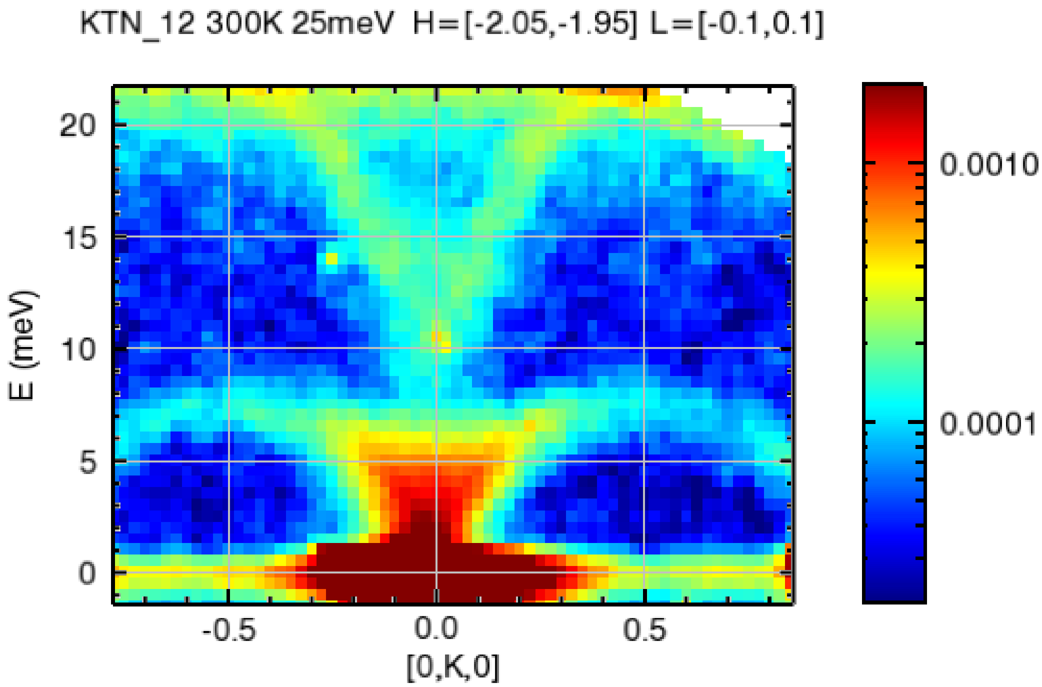


Figure: Transverse acoustic and optic phonon branches in KTN12 along [0,k,0] at 300K.

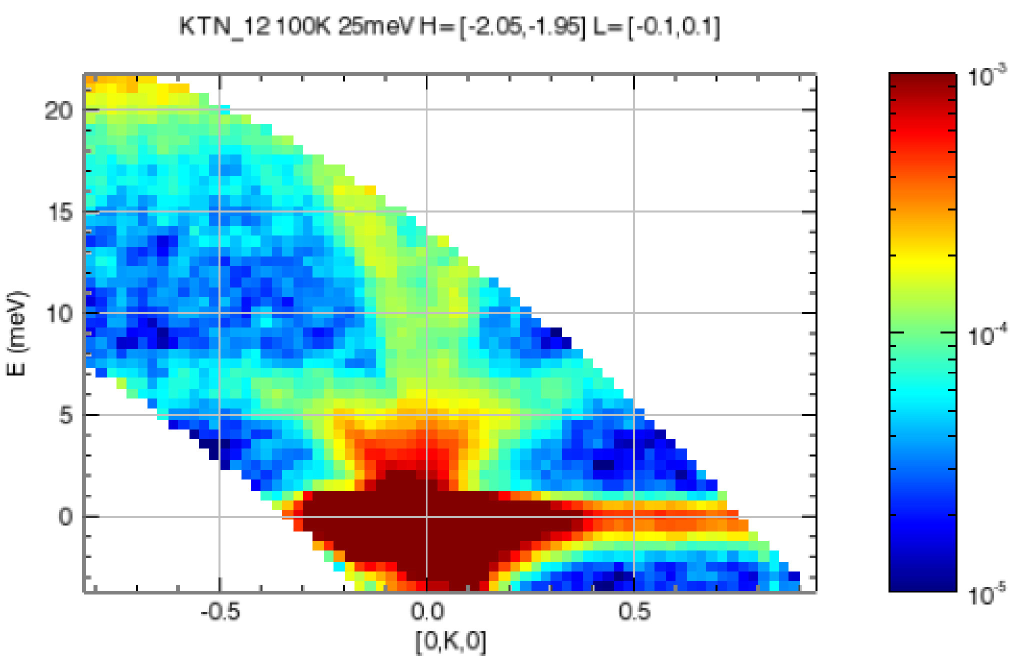
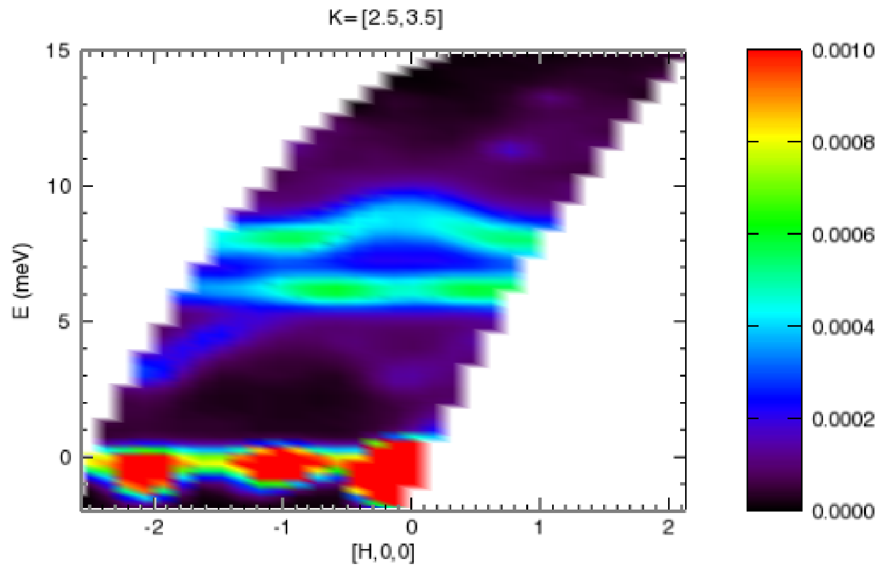


Figure: Transverse acoustic and optic phonon branches in KTN12 along [0,k,0] at 100K.

W. Tian (IPTS-8014, Sep 12-16):



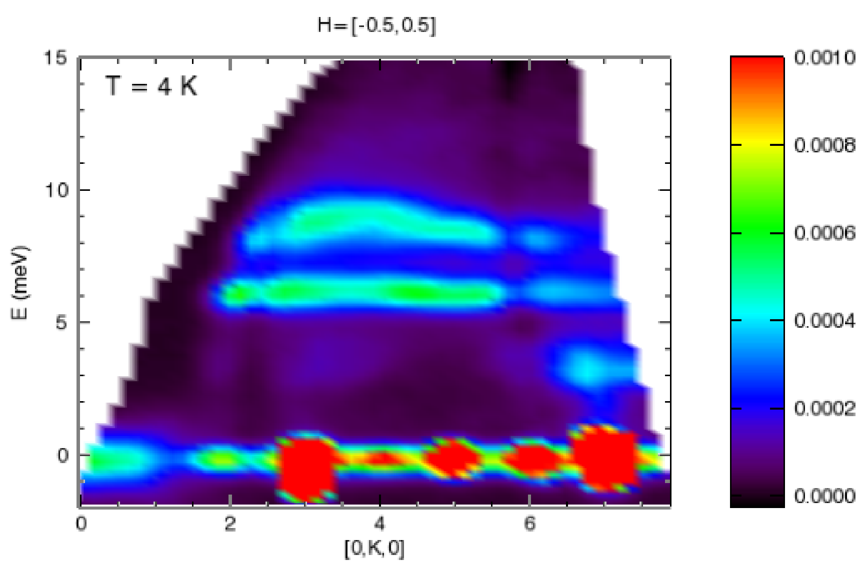


Figure: Tb5Ge4 single crystal measured at 4K using HYSPEC in the [H K 0] scattering plane. Scattering intensity vs. energy transfer projected along the (a) (H 0 0) and (b) (0 K 0) directions. Two spin wave excitations at ~ 3meV and 9 meV were observed. Strong dispersion is observed along the (H 0 0) direction consistent with the magnetic structure of Tb5Ge4.

Zheludev et. al. (IPTS-8004, Sep 17-25):

We had an opportunity to use HYSPEC spectrometer during its commissioning stage in our studies of disordered low dimensional magnetic system. Although we did not manage to perform all the expected measurements due to several reasons (including mercury leak from the target) we were able to experience the performance of the spectrometer. In short, we have found it to be a promising instrument however several issues need attention.

We found the combination of Bragg focusing optics to be a very attractive idea due to significant flux enhancement. However, we had severe problems with background as can be seen in the ‘’instrument view” of Figure1 and the spectrum in Figure 2. In addition, when performing the experiment we would have appreciated having relaxed collimator (80’) present in addition to the very tight ones. Finally, we felt that the shielding around the sample should be improved.

Despite the above mentioned shortcomings which led to us having to use very narrow slits and heavy shielding, we still managed to see the magnetic excitation we were interested in (Figure 3). This serves as a proof that the flux at the instrument is high and that the instrument has good potential.

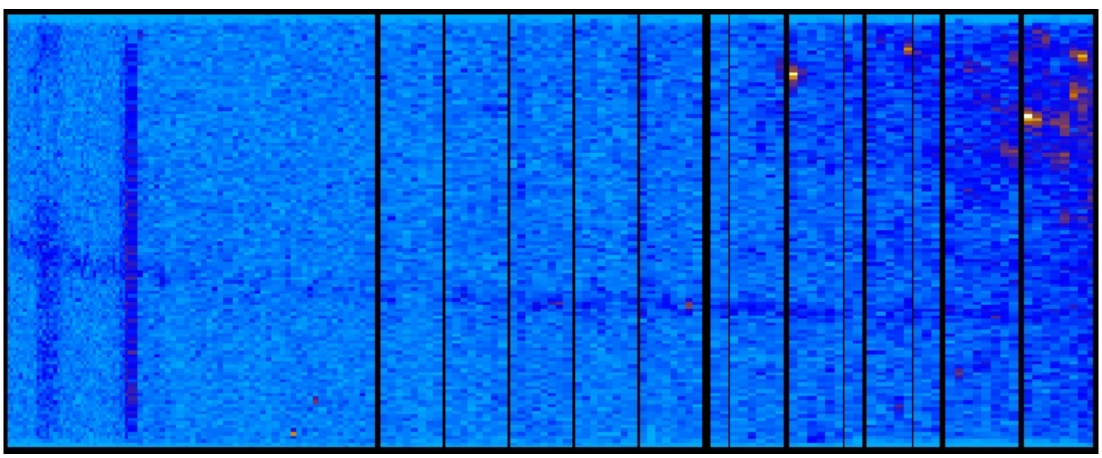


Figure 1: Instrument view of our experiment indicating various background features.

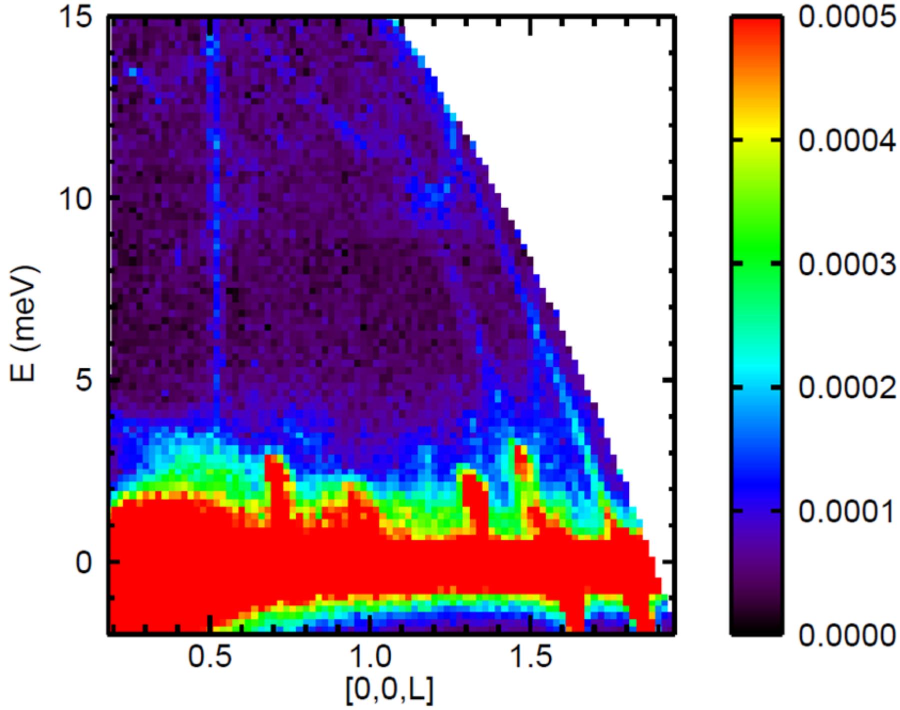


Figure 2: Spectrum with slits set to standard dimensions showing high background.

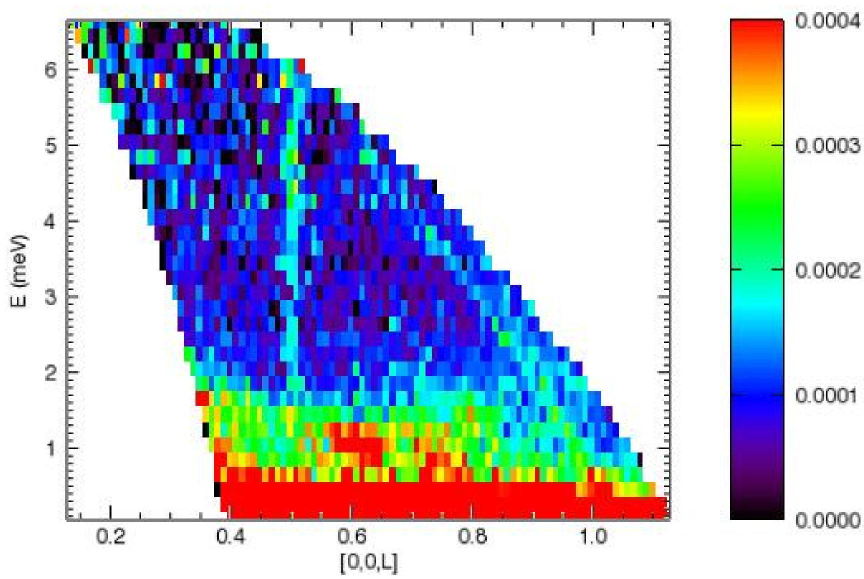


Figure 3: Spectrum obtained with very narrow slits and increased shielding.

Greven (IPTS-8809, Dec 7-12):

This commissioning experiment will study the quantum percolation system La2(Cu,Mg,Zn)O4, using a very large multicrystal sample with ~30% dilution. The idea was to map out S(q,w) as a function of temperature, extending the previous work on the instantaneous structure factor S(q)[4]. The question for HYSPEC was how to work with a large sample and a low detector vessel angle, and how to mitigate background features in this configuration. We did determine that the incident beam was scattering off of aluminum downstream of the sample by ~0.8 m, past the fine radial collimator. Our new shielding and beam stop, along with additional cadmium shielding inside the detector vessel, will hopefully reduce this background feature going forward.

[4] Science v 295 p 1691 (2002)