Response to the 2017 Review of the Instrument Suite for Spectroscopy

September 17–18, 2020

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Response to Recommendations from the 2017 Suite Review

The 2020 instrument suite review is the second triennial review of the spectroscopy suite with the prior review being held November 14-15, 2017. There were both overall and instrument specific recommendations given in the 2017 report. In this document, we summarize responses to these recommendations. The comments from the 2017 reports are in gray and our responses are in red.

Overall Recommendations

Triple-Axis Spectroscopy: "*… these instruments have not progressed from their basic design for many years and now lack capabilities realized in modern multiaxis crystal spectrometers at other facilities worldwide. This has led to missed scientific opportunities for the U.S. neutron scattering community. The committee recommends short-term upgrades of these instruments as indicated in the individual instrument sections. In the longer term, however, we recommend that the opportunity provided by the planned HFIR Be replacement be exploited such that new thermal instruments be optimally designed and installed so as to re-establish international leadership in thermal TAX capabilities at ORNL.*"

Plans have been developed to upgrade the three thermal triple-axis spectrometers (HB-1A, HB-1, and HB-3). The incident monochromators and second monochromator drum on HB-1A (FIETAX) have been replaced providing a 3x increase in flux on sample. A project is underway to rebuild the secondary spectrometer to take full advantage of the vertically focused beams. We are pursuing options to replace the Heusler monochromator on the HB-1 polarized triple-axis spectrometer (TAS). A project is underway to incorporate a velocity selector on HB-3 but, to avoid excessive instrument downtime, the installation of this device has been delayed until the planned Be reflector outage.

Triple-Axis Spectroscopy: "*The capability for cold neutron spectroscopy on CTAX is quite limited at present due to its position on the cold neutron guide, and is far from state-of-the-art. The plans for the new cold neutron triple axis spectrometer (MANTA) which would establish international prominence in this area, are therefore highly recommended*."

The neutron guides and instrument configuration within the HFIR guide hall has been reoptimized to incorporate new capabilities including the MANTA spectrometer and a new neutron spin echo instrument. The MANTA team now includes Adam Azcel, Barry Winn, and Garrett Granroth and we are working closely with Martin Mourigal as the community representative. Garrett was brought into the team recently and has led the neutron optics optimization for MANTA which is nearing completion. Flux estimates for this instrument suggest performance similar to the ThALES instrument at ILL, the world-leading cold-neutron triple-axis spectrometer.

Triple-Axis Spectroscopy: "*Access to and technical support for sample environment apparatus, especially as it relates to very low temperatures and high magnetic fields, is currently significantly limiting productivity at HFIR. The triple axis instruments tend to carry out numerous parametric studies, and the burden associated with reliability and technical support of sophisticated sample environments under these conditions is high. The case was made that this area is under-supported compared with related, successful efforts at European neutron sources. Low temperature and magnetic field/pressure cell capabilities are likely to be more important in the future; especially if a* *state-of-the-art cold neutron triple axis spectrometer becomes available*."

The number of sample environment staff directly supporting low temperature / high magnetic field experiments remain the same as in 2017. Despite this, multiple steps have been taken to increase operational efficiency for these experiments at both HFIR and SNS:

- Despite significant turnover in sample environment (SE) staff we have maintained four staff positions dedicated to supporting high B / low T experiments at HFIR. A dedicated team now provides support for high pressure experiments at both HFIR and SNS.
- Scientific associate (SA) staffing levels at HFIR have increased and training of instrument staff to perform certain sample environment activities has been performed. Examples include sample changes in CCRs, cryostats and cryomagnets and cryogen fills.
- There is now a standard weekend model where one SA and one SE staff member perform cryogen fills. Instrument scientists have also been trained to perform cryogen fills as needed.
- Instrument teams and SE staff now have a clearer mutual understanding of expectations for support
- Cross training of sample environment staff between HFIR and SNS allows resources to be rebalanced as demand changes.
- Block scheduling of complex equipment has now become routine and minimizes equipment moves
- Instrument hall coordinators (IHCs) are now supporting HFIR operations as well. The IHCs become a central point-of-contact for weekend / after-hours support and SE staff have been responsive to their calls for support.

Significant progress has been made in sample environment automation:

- Auto needle valve control is now implemented across HFIR and SNS
- A liquid helium autofill (LHeAF) system was patented in 2018 and licensed to ARS in March 2019. These systems have been used at several SNS instrument and are working on two cryostats at HFIR with plans to expand to other sample environment equipment.
- A multi-point LHeAF system is in the development stage. This will allow multiple instruments to be filled from a single dewar which can be particularly useful with the space constraints of the HFIR beam room.
- The low-T / high-B steering committee (chair: Barry Winn) and high pressure steering committee (chair: Yan Wu) continue to provide a venue to advocate for additional resources (both equipment and/or staff).
- The demand for ultra-low temperature (dilution / 3He inserts) and magnets continue to increase at HFIR and SNS. We have invested in new equipment since 2017 and a complete list of low T / high B sample environment equipment can be found at https://neutrons.ornl.gov/sample/subpage/low-temperature-magnetic-fields. For HFIR (the

focus of this comment in 2017), there are now two ^3He inserts, three dilution inserts, and 12 wet cryostats (increased from 6 in 2017). New cryomagnets at HFIR include an 11T horizontal field magnet (SANS), a 5T horizontal field warm bore magnet (SANS), and a 6T vertical field asymmetric magnet (this magnet will replace an existing old 5T magnet). In addition, an 11T magnet that transitioned from Brookhaven is no longer functional and has been replaced by an 11T magnet that was received from Los Alamos (can only be used at CTAX).

Despite these investments, demand (particularly for cryomagnets) continues to exceed the inventory. To address this, a proposal is being considered to procure an additional 6T vertical field cryomagnet for HFIR.

Direct Geometry Spectroscopy: "The oversubscription rate for ARCS, SEQUOIA, and CNCS is high, but it is particularly high for CNCS. While this is a sign of success, it also makes it difficult for the user base to construct meaningful plans for cold neutron spectroscopy at SNS. The development of the Second Target Station at SNS will help with this very high demand for cold neutron spectroscopy, but that will not be part of a user program for a decade. This further makes the case for a forefront cold neutron triple axis capability at HFIR in the immediate future."

As mentioned above, plans are underway to design and, ultimately complete the construction of the MANTA cold neutron triple-axis spectrometer. The CHESS spectrometer proposed for Second Target Station (STS) will provide world leading capabilities and we are preparing an instrument concept for an extreme environment spectrometer / diffractometer at STS. Unfortunately, none of these will be complete in the short term and, consequently, high demand remains a problem.

Direct Geometry Spectroscopy: "*The data sets associated with single crystal time-of-flight spectroscopy are very large. Good progress has been made in automating data reduction and visualization. However, the ability of user groups to intelligently negotiate large data sets, and to fit their data to meaningful theoretical models, is a significant obstacle to the ultimate productivity of the instrument suites. This is what is required to get to the important underlying science and hence to high impact publications. Additional emphasis on user support in this area, particularly with embedded data analysis expertise is a high priority.*"

Python based routines have been developed within the Mantid platform to combine and visualize data sets obtained from single crystals on the direct geometry spectrometers. These routines perform proper statistical weighting of runs (even when combined runs have differing count times) and have performance gains over currently used software. The lead developer of these routines, Andrei Savici, has recently been hired as the computational instrument scientist in the Direct Geometry Team. Yongqiang Cheng has also been hired as a computational instrument scientist in the Chemical Spectroscopy Team. He has developed tools for calculating lattice dynamics and the resulting inelastic neutron scattering response from first principles calculations from both polycrystalline and single crystal samples. These tools work for both indirect and direct geometry spectrometers. With both Andrei and Yongqiang in the Spectroscopy group, they serve the role of embedded data analysis experts that can work with users.

Chemical Spectroscopy: "*Since JCNS (Jülich Centre for Neutron Science) will stop supporting the NSE instrument in 2020, the committee strongly recommends assessing the future possibilities for this instrument and its role within the DOE/ORNL mission as soon as possible to ensure a smooth transition in 2020. Further discussions can be found in the section on NSE*."

The NSE instrument is in the process of transitioning to ORNL operation. Current status of the staff on NSE:

1. Instrument scientist Laura Stingaciu and Scientific Associate Mary Odom are employees of ORNL
2. Instrument scientist Piotr Zolnierczuk is still employed by the Juelich Center for Neutron Science; he has signed an ORNL employment offer and will transition to ORNL staff in Dec. 2020.

Chemical Spectroscopy: "*It was noted that the beamtime allocation across all three instruments is not as effective as it could be. The committee suggests increasing the flexibility in scheduling beamtime and streamlining the safety reviews to fully optimize beam usage. It is duly noted that a rapid access mode exists at SNS, however this rapid mode still takes too long to be truly flexible. We suggest generating "super"-rapid access for time-sensitive measurements that cannot easily wait a few days. It is also highly beneficial for the productivity of the beamlines to allow for more discretionary time for proof of principle experiments and general testing. Discretionary time can also successfully be used to complete missing datasets for experiments that got cut short due to loss of beam or malfunctioning equipment. The completion of experiments often leads from an unusable dataset to publishable data.*"

There are different categories of beamtime that can address most of the concerns above. Proof-of-principle beamtime exists with limitations of 1 day per allocation. Commissioning time is available to test new equipment and capabilities. There are now two components to discretionary time – a fraction of the time is allocated by the science initiatives and the other fraction is at the discretion of the instrument team. Programmatic proposals have been replaced by Collaborative Development proposals designed to focus on user program capability development. Instrument teams can continue a general user proposal which has already been completed when additional time is required. A process for expanding the mail-in program has been developed and we are preparing to implement a mail-in program on VISION initially followed by ARCS. Director's discretionary time exists for projects of high importance that need to be scheduled and allocated quickly.

Instrument Specific Recommendations

Triple-Axis Spectroscopy

Comments applicable across the triple-axis instrument suite:

"The level of sample environment support is inadequate, and this leads to loss of efficient beamtime, especially during evenings and on weekends. This level of support is not at an internationally competitive level. Backup equipment in the event of a sample environment failure is not always available."

See the discussion in the "Overall Comments" section.

HB-1 (PTAX)

Specific suggestions provided to bring polarized triple-axis performance to an internationally competitive level:

"The complete refurbishment of the Heusler crystal optics at a state-of-the-art level is a priority. This upgrade should target flux/sensitivity levels where any reasonably sized sample (≈ 1 – 2 cc) measured on the other instruments could be brought to HB1 to obtain more detailed information on its magnetic properties (detection of inelastic magnetic scattering and information on its anisotropy)."

A science productivity proposal was submitted and approved to obtain new Heusler crystals for the HB-1 monochromator. Discussions are underway to determine the optimal source for these crystals.

"The primary spectrometer mechanics should be improved such that the monochomators can be changed without the use of a crane."

The recommended mechanism is technically challenging because the space inside the monochromator shield is limited. The mechanism requires a considerable redesign of the monochromator shield and plug, which would not be feasible in the near future. In the meantime, we strive to schedule polarized and unpolarized experiments efficiently to minimize the impact of having to manually change monochromators.

"Performance benchmarking with respect to the PA capabilities of HYSPEC as well as to polarized TAS instruments worldwide (in particular the ILL instruments IN20, IN22) should be carried out."

Due to the unexpected HFIR shutdown and the COVID-19 pandemic, we have had no chance to perform a benchmarking test of our polarized neutron setup. In the near future, we would like to measure the same sample at HYSPEC and HB-1 to get an idea how the two instruments can be used in a complementary way. We plan to measure spin wave excitations of a $BiFeO_3$ single crystal, in which we expect strong magnetic excitations in a wide energy range (<70 meV). We also plan to measure magnetic and lattice excitations using crystal of MnO, which is used to demonstrate the separation of magnons and phonons. In order to directly compare HB-1's PA capability with those of other instruments worldwide, we will measure HB-1's absolute neutron flux using gold foils.

HB-1A (FIE-TAX)

"A development plan exists to automate and modernize both the sample and analyzer portion of the instrument … The double-bounce monochromator system could be upgraded to enable the incident energy to be changed, which would greatly expand its capabilities both for diffraction and some inelastic scattering where good signal-to-noise is needed."

Careful analysis of the vertical focus on HB-1A identified an overfocused beam which reduced the flux on sample. A project was initiated and completed to address this problem. This is still a single incident wavelength instrument, but the monochromator upgrade resulted in a 3x increase in flux on sample. A project is underway to modernize the secondary spectrometer of HB-1A.

HB-3 (TAX)

"The installation of a velocity selector to allow a clean monochromatic beam at a range of energies to impinge on the sample is planned and should be the highest priority for this instrument."

A project was initiated to design and procure an incident beam velocity selector for HB-3. Accommodating this device requires redesign of the instrument beam shutter and the shields around the monochromator drum to reposition the monochromator slightly downstream. Due to the schedule for this work and the long down time to complete the project, the decision was made to defer installation until the Beryllium reflector change.

"Improvements such as motorized beam-size limiters, and sample enclosure, to reduce ambient radiation fields and improve signal-to-noise, to reduce crosstalk with other nearby instruments, and to reduce personnel radiation exposures, would be improvements."

We recently installed shielding around the HB-3 sample table, which consists of two trains of shielding panels moving along the track as S2 changes. The omega-shaped track has its open ends attached to the monochromator drum. The train lengths are configurable by adding or detaching links (panels). The entire train can also be disconnected from the S2 arm and rolled away for introducing sample environment equipment or other necessary access to the sample area. This would also be necessary when driving the S2 arm to high angles allowing for the full range of S2. The preliminary test has shown that the new shielding cuts neutrons and Gamma radiation by half. It also significantly reduced instrumental background on neighboring instruments. More reduction of the radiological background is expected when we have Flexi-boron sheets attached to the other side of the panels.

"The analyzer system for HB3 is antiquated and modernization would greatly improve the quality of the data, allowing more challenging science to be successfully explored. In particular, upgrading the energy analysis system to allow variable energy double focusing, or configurations utilizing a position-sensitive detector, found in modern triple-axis style spectrometers, would provide new and valuable measurement capability."

A preliminary design for a new secondary spectrometer has been developed that incorporates a multiplexed analyzer-detector system, in which the existing single detector will be replaced by a radial array of linear position sensitive ^{3}He detectors, centered on the sample center. It encompasses a viewing angle of 16° from the sample position. The central portion of this array is well shielded and functions as the former single detector did. This effective single detector is used in the conventional flat analyzer single detector mode and monochromatic point-to-point horizontal focusing mode. The PSD portions of the array lie on both sides of the single detector portion, on a smaller radius. These detectors are used along with the single detector group for diffraction using the PSD, and monochromatic q-dispersive mode in transmission geometry. The existing fixed analyzer will be replaced by one that has translatable, rotatable "spines" (curved columns of PG crystals), enabling operation of the instrument in the horizontal focusing geometry or a dispersive mode.

CG-4C (CTAX)

"The future of cold neutron spectroscopy at ORNL is a key to the overall success of the mission of Neutron Sciences. The succession plan for cold neutron TAX at CTAX is the plan for implementing MANTA, the new triple (multi) axis spectrometer. Such a capability will indeed establish cold neutron TAX spectroscopy as a world leading capability, and the user demand in the area is great. For these reasons, the development of MANTA is highly recommended."

"It is highly recommended that MANTA be realized in next five years. It will be important for CTAX to be available and functioning as well as possible until MANTA is available to the user program. After that point, CTAX can be decommissioned."

MANTA is a key component of the redesigned HFIR cold guide hall. The team working on MANTA has been expanded to include Barry Winn and Garrett Granroth and Garrett has taken the lead in designing the incident beam optics. Current McSTAS simulations suggest performance similar to ThALES at ILL making it a world leading instrument. CTAX will indeed cease to operate after the beryllium reflector change at HFIR. Initial operation of MANTA will utilize the CTAX secondary spectrometer and this will also be used for certain measurements (for example, Wollaston prism and polarized experiments) after completion of the multi-analyzer secondary spectrometer.

Direct Geometry Spectroscopy

BL-5 (CNCS)

"Short term instrument developments are well planned out and absolutely necessary. Expanding the detector coverage should be of high priority. A new radial collimator is set for installation and this will be used with the larger cryomagnets. We feel that polarization analysis on CNCS is not a priority, as HYSPEC will be the venue of choice for these developments and experiments. Returns on a T0 chopper and Rep-rate multiplication are thought to not be commensurate with the investment required."

A project is underway to incorporate detector tubes obtained from PHAROS on CNCS. This will expand the out-of-plane detector coverage substantially. The new radial collimator is operational and works well to reduce background. It is compatible with our cryomagnet inventory including the new 14 T magnet. As recommended in 2017, we have not further pursued either polarization analysis or rep-rate multiplication on CNCS.

"For the longer term (~10 years) several cold TOF instruments will become available that will outperform CNCS in sheer numbers of flux and resolution, in particular instruments planned at ESS and also at STS. This raises the question of the scientific future of the CNCS instrument. The instrument team is well aware of this and has discussed options for CNCS to continue an important role by changing its mission. Among the possible options noted are to shift to a soft matter/ chemistry heavy scientific mission, for which it will continue to provide fully adequate intensity and resolution. Another possibility would be to continue studying hard matter but with large samples (as most new instruments will be designed for small samples). Either scenario is well founded and would allow CNCS to continue to be a world leading instrument, although perhaps in more niche areas."

We are pleased that the 2017 committee recognized the long-term plans for CNCS and see the value of this spectrometer even with future developments at both HFIR and STS. We are continuing to develop plans for instruments such as CNCS as the instrument selection for STS is finalized.

BL-14B (HYSPEC)

"There is good evidence that the instrument team have a good grasp of what is required to turn HYSPEC into a solid DGS with polarization analysis. They need time and support to concentrate on further characterization of their supermirror analyzer, and development of operational matters (such as interchange of the analyzer, oscillation, XYZ vs Z PA vs 10pt). They have a good grasp of what is required in terms of outreach (viz. PNCMI 2016) - and these efforts are crucial to expand their user base."

The supermirror array which was on loan from the Paul Scherrer Institut was purchased by ORNL in the summer of 2020; this is the largest investment at HYSPEC in the 2017-2020 period. Detailed characterization of the supermirror performance has been performed, and strategies for more efficient data collection have been identified. The XYZ polarization analysis mode has been used at HYSPEC extensively over the past three years, and the ability to capture diffuse inelastic features with polarization contrast distinguishes HYSPEC worldwide. The most important change since the 2017 review was the installation of the oscillator / elevator system in August of 2018. This system was approved in the fall of 2016 as part of the scientific productivity program. The oscillator significantly smoothed out transmission for the supermirror array and the oscillator mount for the supermirror enabled modest alignment corrections. Furthermore, the elevator feature both simplifies and speeds up our transition from unpolarized to polarized and back, which has enabled users intending to leverage polarization capabilities to quickly convert to unpolarized as needed, and has simplified the block scheduling process since we no longer have to block polarized experiments together. In addition to the physical improvements for polarization analysis, the HYSPEC team has also improved the reduction workflow, with a strong involvement from colleagues from Brookhaven National Laboratory.

"They have specifically asked about whether they should include ^{3}He analysis and a supermirror polarizer in their future upgrade planning. Our recommendation is that - for now - they should focus their efforts on optimizing the supermirror analyzer - concentrating on cold neutron spectroscopy where the analyzer functions best. At the same time a close eye should be kept on wide angle 3He developments at NIST and MUNICH (SEOP) and at ILL/ISIS/ANSTO (MEOP). There is a good possibility that in the future, a mature version of a wide angle 3He device will be available to purchase and install."

As recommended, the instrument team has focused on optimizing operations utilizing the supermirror analyzer.

"We see no convincing case for the addition of either a supermirror polarizer, or a radio-frequency flipper, in the primary beam. The addition of a wide-angle flipper before the supermirror array would be a valuable addition – but it should be noted this has previously been tried at DNS and D7, and was found to be technically very challenging. Further investigation of this is recommended but may require significant resources to achieve."

With the knowledge and expertise accumulated by the HYSPEC team over the past years of operation it became evident that there are notable benefits from adding a radio-frequency flipper. In addition to the improved transmission, anticipated improved flipping ratio and simplicity (no flip current optimization required for different incident energies) compared to the currently-used Mezei flipper, a RF Flipper also affords the opportunity to cross calibrate both the Mezei and the RF flippers and to determine the polarization of the other HYSPEC optics. With the support from NSD and RAD staff an optic-rail mounted RF flipper was designed and built. In addition, a compact 3D coil system was fabricated to enable more flexibility when planning for future polarization developments. The HYSPEC team has prepared an advanced draft for an ORNL SEED money proposal and is currently evaluating the feasibility of two different flipper technologies for this flipper. If successful we will then have the first wide-angle white-beam flipper anywhere compatible with a polarizing supermirror array.

"It is commendable that efforts are being pursued in the direction on Spherical Neutron Polarimetry, and half-polarized setups. It is to be noted nevertheless that these techniques (when combined with spectroscopy as opposed to diffraction) are not generally in high demand. Before embarking on these programs, the instrument team are encouraged to build a solid science and business case for these efforts."

In support of LDRD 8824: "Portable High-Tc Wide-angle Spherical Neutron Polarimetry Device" led by Peter Jiang and with Barry Winn as collaborator, a spherical neutron polarimetry system (SNP) intended for use at both HB-1 (PTAX) and GP-SANS at HFIR was tested at HYSPEC in December 2019. This commissioning experiment followed an initial direct beam configuration test at the University of Missouri Research Reactor. The HYSPEC test demonstrated the use of both variable scattered beam directions and successful operation with a narrow tail wet cryostat. In addition to demonstrating SNP, this test enabled the LDRD team to identify several improvements which will enable the SNP to operate more robustly at HFIR. Finally, the success of this LDRD motivated a successful application for a DOE Early Career Award for Peter Jiang, in which Ovidiu Garlea served as mentor / scientist.

The half-polarization technique has been used successfully in the user program for studying magnetization density distribution and spin dynamics in saturated ferromagnets, ferrimagnets and paramagnets under modest applied magnetic field obtained with vertical or horizontal permanent magnet yokes. While several lessons have been learned that provide useful clues for future studies, the performed experiments have led to 5 publications and are expected to grow and diversify the HYSPEC user base. Ovidiu Garlea's productive collaboration with Michael Shatruk of Florida State [a-c,e], benefits from this powerful technique.

[a] X. Tan, V.O. Garlea, P. Chai, A.Y. Geondzhian, A.A. Yaroslavtsev, Y. Xin, A.P. Menushenkov, R.V. Chernikov, M. Shatruk, "Synthesis, crystal structure, and magnetism of $A_2Co_{12}As_7$ (A=Ca, Y, Ce-Yb)", *Journal of Solid State Chemistry* **236**, 147–158 (2016).

[b] X. Tan, Z.P. Tener, M. Shatruk, "Correlating Itinerant Magnetism in RCo_2Pn_2 Pnictides (R = La, Ce, Pr, Nd, Eu, Ca; Pn = P, As) to Their Crystal and Electronic Structures", *Accounts of Chemical Research* **51**, 230–239 (2018).

[c] J.K. Clark, X. Tan, V.O. Garlea, A.A. Arico, A.P. Ramirez, V. Yannello, C.M. Thompson, K. Kovnir, M. Shatruk, "Reentrant spin glass state induced by structural phase transition in $La_{0.4}Ce_{0.6}Co_2P_2$", *Physical Review Materials* **4**, 074412 (2020). (see the final HYSPEC highlight)

[d] Y. Nambu, J. Barker, Y. Okino, T. Kikkawa, Y. Shiomi, M. Enderle, T. Weber, B. Winn, M. Graves-Brook, J. M. Tranquada, T. Ziman, M. Fujita, G. E. W. Bauer, E. Saitoh, and K. Kakurai, "Observation of Magnon Polarization," *Phys. Rev. Lett.* **125**, 027201 (2020).

[e] Z.P. Tener, V. Yannello, J. Willis, O.V. Garlea, M. Shatruk, "Magnetization Distribution in $Cu_{0.6}Mn_{2.4}Ge_2$ Ferromagnet from Polarized and Non-Polarized Neutron Powder Diffraction Aided by Density-Functional Theory Calculations," *J. Magn. Magn. Mater* (2020, in press)

BL-17 (SEQUOIA)

SEQUOIA has identified three major improvements, all of which will contribute to substantially greater impact. These are:

1. the acquisition of a radial collimator to allow for large and sophisticated sample

environment, such as magnet cryostats and pressure cells on SEQUOIA.

An application for funding was submitted for an oscillating scattered beam radial collimator for SEQUOIA in September of 2017 through the Science Productivity Program (SPP). The project was A-Listed and approved in this program on October 18, 2017. Funding was never awarded to this project due to critical needs for other instruments in the directorate. Monte-Carlo calculations have been performed to place the collimator inside the detector tank. It was determined that this would shadow the top row of detectors.

2. Filling out SEQUOIA's complement of position sensitive detectors thereby making SEQUOIA much more efficient.

   SEQUOIA has purchased six detector 8-packs since 2017. Four of these have been installed, one of these is being procured, and one of these is being assembled in the summer of 2020. Applications for Midscale Instrument Improvement money to purchase larger groups of detector 8-packs have been submitted in 2019 and 2020.

3. The incorporation of a low angle detector bank to enable Brillouin scattering (relatively high energy transfers at low wavevector transfer).

   An application for funding was submitted for the Brillouin scattering detector upgrade for SEQUOIA in September of 2017 through the Science Productivity Program (SPP). The project was A-Listed and approved in this program on October 18, 2017. Funding was never awarded to this project due to critical needs for other instruments in the directorate.

BL-18 (ARCS)

"Specific recommendations for improved performance are to:

1. Replace the data acquisition system.

   The data acquisition system has been replaced by the EPICS / CSS based system employed at other beam lines. This is now utilized on all scattering beam lines at SNS.

2. Develop and deploy a multi-sample changer for samples at room temperature and below.

   ARCS has completed a design and is waiting for manufacturing to implement a multi-sample changer that would use the existing large bore CCR and add a motorized 6 sample stick. One rotation and one vertical translation will allow samples to be positioned in the ARCS beam. To fit within the existing CCR and use the entire ARCS detector array without interference, the design uses a new 3D printing technology to make the sample mount from a B4C/aluminum composite. This combines the support and heating requirements with neutronic shielding for a compact design. The initial temperature range is planned for 10K to 450K and testing of a mock-up holder is underway to understand the thermal impact on cooling and heating of the larger holder in the CCR.

3. Complete an analysis of the benefit of a disc chopper for energy resolution improvements that could improve dynamical pair distribution function analysis.

   A study of the scientific justification and technical requirements for an additional chopper at ARCS has not been completed. Initial considerations for the use with incident energies up to 200 to 300meV to reach the desired Q range for dynamic PDF measurements indicate it would be based on the current Fermi chopper design. Evaluation is needed to see if additional shielding mass could be added to the current payload to improve overall background suppression. Specific requirements for the Fermi slit package await a detailed study of the resolution improvement versus intensity reduction compromise. Additional advantages for an improved resolution option at ARCS include better measurements of the phonon dispersions across the entire Brillouin zone to enable more detailed study of thermodynamics in single crystals. The loss in intensity would be offset by higher source power and improvements in data folding techniques to optimize the use of the full ARCS data set. Some improvements that are more difficult to quantify would be a more symmetric energy resolution shape and suppression of background from neutrons that pass the T0 chopper but then scatter within the neutron guide and shielding but make it through the current Fermi chopper.

Chemical Spectroscopy

BL-2 (BASIS)

"Continue to refurbish the Si (111) detector tanks (2 of 4). The instrument scientist has already replaced one detector bank and shown that the resolution function has been significantly improved. This improvement can better the quality of data close to the elastic line for weak scatters or samples with slow dynamics."

The current cost to get the two (out of three) Si(111) analyzer quarters refurbished is estimated at between $1,250,000 and $1,500,000. In view of this, an effort has been made to provide users with both "high intensity" and "high resolution" data reduction options and let them decide whether the loss of two thirds of the counting statistics warrants the resolution improvement for their data sets. The fourth, Si(311), analyzer quarter, is fully operational. An innovative approach of utilizing Si(333) reflection from the existing analyzers has been proposed and tested.

"Finish testing the BWAVE prototype (roughly $150K, 1 week of beam time). This work is critical to the strategic plan of STS. A successful demonstration of the concepts presented in the design of BWAVE is critical to ensure the preeminent leading role of ORNL in QENS/INS."

Funds were committed from the Spectroscopy group to complete testing of the BWAVES prototype. Final testing has not been completed because it requires commitment of the specific staff in the Chopper group (NTD division), which has not been authorized to date.

"More effective beam time use could be achieved by the following:

a) Increase the flexibility of the use of the beam-time, such as changing experimental plans or samples on the fly, contingent upon the approval of the instrument team and the safety team. Flexibility in adjusting the use of beam-time within the frame of the user program is necessary to run an instrument more effectively."

   It is the goal of NSD staff to efficiently and effectively use neutron beam while ensuring the integrity of NScD's General User Program (GUP). NSD does allow some deviation from the experimental plan and samples set forth in the approved proposal. However, it is important that the changes do not a) conflict with other approved proposals creating a potential conflict or b) create an unreviewed safety hazard. Users are strongly encouraged to contact their local contact immediately if they desire to make sure changes so they could be reviewed for conflicts or changes. It is difficult to accommodate proposed changes that are not discussed with the local contact prior to the start of the experiment.

b) Having safety review streamlined and extend the period of safety review validity.

   NScD has a robust environmental, safety and health program the complies with a variety of laws, regulations and standards and ensures the safety of staff and users. All proposals are reviewed for feasibility and operations. These reviews check to determine if the hazards the proposal presents can be properly controlled and mitigated. Once the safety review has been completed and ES&H staff have signed the experimental safety summary (ESS), this safety review is valid for

6 months to allow for follow-on measurements as required. Users are provided on-line training prior to their arrival at ORNL. When on-site users receive beamline training, they sign the ESS which outlines the controls necessary to protect the user and others during their experiment.

User training is continuously reviewed to ensure that only the relevant information is provided to the user. Since 2017, the on-site practical factors training was streamlined to only require demonstration of the use of radiological instruments.

c) Allow more discretionary time for proof of principle experiments, testing, finishing experiments. Allow "super"-rapid access to allow time-sensitive measurements.

Proof-of-principle experiments can be allocated as needed for either discretionary or general user experiments. Finishing of experiments can be accomplished through a continuation process. A director's discretionary time mechanism exists to support time sensitive experiments. Requests for time using this mechanism are rare and, consequently, this method seems adequate to address such rapid access requests. NScD's Industrial Applications Program works with industry users that may require rapid access because of an emerging issue that may be impacting their operations.

d) Continue to improve ancillary equipment such as the polarization capability.

It was determined that a ^{3}He cell would provide a suitable polarization solution for BASIS. Given the very challenging geometry of the BASIS sample well, a major design effort would be required to address this challenge. No progress has been made since the LDRD project that was supposed to support this design work was not funded.

"Hire one extra staff member to assist modeling and simulations. This could potentially lead to publications with even higher impact."

Yongqiang Cheng has recently transitioned to a role as a "Computational Instrument Scientist" on the Chemical Spectroscopy Team. He will provide support to BASIS, VISION and NSE. As part of the ICEMAN project, data analysis capabilities, QClimax, were developed for QENS data analysis. The BASIS team is actively involved in the ongoing development of QClimax.

BL-16B (VISION)

"ORNL should hire a third instrument scientist with chemistry or related scientific background and good experimental skills to assist users with the practical part of the experiments. Thanks to the high flux, spectrometers like VISION are now becoming high-throughput instruments that are attracting users with more and more complicated setups and in-situ or time-dependent runs. This requires expert assistance for the users in the preparation of the more complicated experiments, as well as help in evaluating data as it is acquired to make decisions on the spot regarding the course of an experiment. With run times of the order of minutes to a few hours, the current level of staffing is not enough to cover user support 24/7 during a run cycle."

A Scientific Associate (Eric Novak with a PhD in Materials Science) has been hired to work on VISION. He was hired in early March and the current work restrictions have slowed his full integration into the instrument team. Additionally, Yongqiang Cheng has transitioned to the role of Computational Instrument Scientist which limits his direct involvement in supporting experiments on VISION. With the current emphasis on simpler, remote experiments, current staffing levels are adequate. Despite this, with an eye to the future, hiring an additional instrument scientist for VISION remains the highest staffing priority for the Spectroscopy Group.

It is worth noting that instrument operations have been streamlined and improved in a number of ways which helps to mitigate the point above:

1. Considerable increase in automation (e.g., CSS, automatic data reduction)
2. The development of documentation has increased user independence;
3. Increased support by sample environment for more complex environments (e.g., pressure cells)
4. An increasing number of repeat users who require less support.

"VISION urgently needs more dedicated laboratory space housing sample characterization equipment (such as BET, FT-IR, XRD, TG/DSC ….) to investigate changes in samples before/during/after beamtime as well as check samples that are synthesized at SNS because they cannot be transported easily. As a start two actions could be taken: a) the chemical fume hood in the VISION lab needs to be installed to allow for handling of chemicals in this laboratory located close to the beamline and b) more space in the chemistry laboratory area on the 2nd floor of the main office building at SNS needs to be claimed to house more equipment supporting SNS (and VISION) users with more sophisticated sample handling needs."

This remains an outstanding issue and little progress has been made. The fume hood in the VISION lab has not been installed. The H-203 2nd floor lab has limited space which restricts expansion. Some equipment has been requested as part of the mid-scale investment call within NSD.

"VISION needs a custom-made CCR with a larger sample compartment to accommodate bigger sample environment equipment. This will open up scientific areas that are currently difficult or impossible to approach, e.g. using magnets or larger pressure cells."

A proposal for a larger bore CCR was submitted to the mid-scale call within NSD. This is designed to allow for more rapid sample cooling which will increase instrument throughput. It would also be compatible with a simpler sample changer which could be designed in the future.

"ORNL should build BeFAST on beam port BL-16A to complement VISION in the high-energy range. Easy to build and operate it will make effective use of the small space between VISION and NSE. BeFAST can supply users of neutron vibrational spectroscopy with the information on stretching modes of molecules, an energy range where VISION has more limited intensity and resolution. Besides complementing VISION, BeFAST will ease the oversubscription at VISION, especially for experiments requiring poorer energy resolution."

BeFAST remains a priority for Spectroscopy and is one of the only concepts that can effectively utilize the BL-16A location. Unfortunately, VENUS and DISCOVER are higher priorities for the division and this, combined with the upcoming HFIR Be reflector change makes it unlikely that this will be completed in the near future.

“The 90 deg. diffraction detector banks must be installed together with the necessary collimators. The corresponding data reduction software must be developed.”

These diffraction detectors and associated collimators have been installed and commissioned. The data reduction software is also complete allowing diffraction patterns to be collected together with vibrational spectra. PDF is being developed, quite successfully.

“User community development efforts ought to be encouraged and supported (workshops, conferences, seminars, etc).”

VISION has produced a number of high impact papers over the past few years. This has not gone unnoticed and appears to be some of the best publicity for the beam line. I frequently get requests from users who want to do the same thing as in some published manuscript or are asking if they can do something similar. The web site highlights help too. Training sessions focused on the use of the OCLIMAX software package have been held to assist users with modeling of VISION data.

“Simplify the beam allocation/run authorization process to take advantage of the flexibility afforded by the VISION high flux, which permits the interleaving of experiments for increased efficiency and productivity.”

See the comments presented above in the BASIS section as related to flexibility and beam allocation.

BL-15 (NSE)

“ORNL should commit to the long term support of the SNS-NSE as soon as possible. The uncertainty regarding the long term status of the instrument might undermine instrument operations, discourage a still developing user community, and sap the NSE team moral.”

Juelich and ORNL agreed on the transition and full operation of SNS-NSE spectrometer by ORNL. The agreement documents have been signed and approved by DOE. The instrument staff have transitioned (or will transition) to ORNL employment during 2020. ORNL is committed to keep the NSE spectrometer in the User Program, developed and fully integrated as an SNS spectrometer.

“The efforts to support the soft-matter user community, both within and outside ORNL, should be continued. Providing both deuteration and data interpretation support (via suitable computing facilities and personnel) specifically tailored for NSE users could be beneficial.”

Extensive effort was put by the instrument team into outreach and expansion initiatives by organizing workshops, participating in neutron schools and neutron conferences to advertise NSE spectrometer and encourage the user community, as well as to train the new generation of SNS-NSE users. Upon the transition to ORNL and having the support of SNS resources the team is looking forward to future endeavors into computing and data analysis support for users specifically tailored for NSE science.

“The new reduction software DRSPINE should be deployed as soon as possible. Current new sample environment development projects should be supported without forgetting the need of the magnetic community. The staffing of the NSE team should be shored up. A plan for timely replacement of the aging instrument components should be devised."

The DRSPINE reduction software has been deployed on the analysis cluster and is available for NSE users.

The SNS-NSE underwent several upgrades over the past years in order to improve the overall instrument performance and broaden the flexibility and capabilities as stated in the *"Update on Instrument Development Activities*" part of the Spectroscopy Suite Review document.

Hard condensed matter and magnetic studies were encouraged over the past 3 years to take advantage of the unique ability of neutron spin echo to distinguish discrete change in the dynamic properties of magnetic charges of permalloys and antiferromagnetic crystals. In a recent study currently submitted to Science, Yiyao Chen and his collaborators from University of Missouri show direct experimental evidence of a new mechanism of electrical conduction in artificial honeycomb lattice of single domain size element.

Our Cryo-Furnace was upgraded to a new sample can better suited for low-temperature experiments and we are look forward into purchasing a new cryostat that will allow millikelvin temperatures. The NSE team in committed to have a hard matter and magnetic user community developed at SNS-NSE.

SNS-NSE Instrument Scientist Piotr Zolnierczuk and co-authors released and published the new dedicated software program called DrSpine (Data Reduction for Spin Echo) to address this issue and presented their results in [J. Appl. Cryst. (2019) 52:1022-1034].

The NSE staff has transitioned to ORNL and there are plans to upgrade the power supply system, the analyzer-polarizer system, and other aging components of the NSE spectrometer. We have now the full support of NSD and SNS support teams.

"Current avenues for experiment feasibility testing should be expanded."

With the help of management and SNS support groups it is now possible to submit short proposals (2~3 days) for SNS-NSE that will test the feasibility of an experiment. Upon the transition of SNS-NSE to ORNL, staff can now have access to discretionary time, that can help test samples during shorter experiments.

"The project of a high resolution NSE spectrometer at HFIR is highly recommended as the best avenue to provide the user community with the possibility to study relaxation processes of the order of hundreds of nanoseconds. This dynamic range is crucial for the soft-condensed matter field. Studies should be started regarding a possible complementary role played by the SNS-NSE alongside a high resolution NSE spectrometer at HFIR."

Following this advice and feedback from the community, a high resolution NSE instrument at HFIR is a component of the plans for a restructured HFIR guide hall. The incident beam optics have been designed for this instrument. The plan forward is to start with the instrument design during the Be reflector change at HFIR.