2017 Review of the Instrument Suites for Inelastic Scattering,
Oak Ridge National Laboratory

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Prologue

The review panel met on site at ORNL on November 14, and 15, 2017, for informational sessions chaired by Dr. Richard Ibberson. The panel was asked to assess the progress and performance of 4 triple axis instruments at HFIR (HB1, HB1A (PhiTAX), HB3, and CTAX) and 4 direct geometry time-of-flight spectrometers at the SNS (ARCS, SEQUOIA CNCS, and HYSPEC). The panel was provided beforehand with information regarding the details of the instrument performance over the recent past, and heard presentations from the staff scientists, with opportunity for questions and discussion. The review panel were asked to complete numerical ratings with commentary on each of the instruments as follows:

1. Scientific Mission and Impact
2. Beamline Productivity
3. Leveraging of specific SNS/HFIR characteristics
4. Effectiveness of beam time use
5. General User Program quality
6. Adequacy and reliability of software, sample environment and ancillary equipment
7. Future instrument science and development plan
8. Overall Recommended Actions including recommendation to NScD for continuation, a re-review *before* three years

Overarching Comments and Recommendations on Triple Axis Instrumentation:

1. The triple axis suite provides excellent capabilities in the U.S. for thermal, unpolarized inelastic neutron scattering with conventional Söller collimation. The scientific productivity for these types of experiments has been high, owing in large part to the superb expertise and dedication of the scientific staff in producing high-impact research.

However, 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.

2. 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.

3. 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.

Overarching Comments and Recommendations for Time-of-Flight Instrumentation:

1. The direct geometry chopper spectrometer suite of instruments at SNS are the world leading capability in this area, and, as a whole, have high productivity. HYSPEC is making excellent progress implementing polarization analysis within a time-of-flight venue.

2. 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.

3. 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.

Instrument Reports – Triple Axis Suite:

HB1 – PTAX

HB1 is a thermal beam, triple axis spectrometer (TAX) offering pyrolitic graphite (PG) and Heusler monochromators/analyzers for unpolarized and polarized scattering experiments, respectively. Configured in its unpolarized mode (PG crystals), it operates well and serves a productive user community; however the polarized setup is outdated (absence of variable focusing, tiny analyzer crystal) such that it only permits primarily diffraction work, technical developments (spin-echo with Wollaston prisms) and occasional inelastic work when sufficiently large sample crystals and strong motivation are available. The beam polarization of ≈ 85% (flipping ratio < 15) is on the lower side of the useful value range. The strategic vision for HB-1 is to be competitive with the best polarized triple axis spectrometers in the world, but it is far removed from this at present. Greater focus on meeting the capabilities of the international suite of competing polarized TAX instruments, such as IN20 and IN22 at the ILL, would be beneficial.

1. Scientific Mission and Impact: 2

HB1 has an important mission to provide some neutron polarization-analysis (PA) capabilities, and thereby complement the unpolarized TAX instruments at HFIR (HB1a, HB3) and direct geometry chopper spectrometers at SNS (ARCS, SEQUOIA). This role is, however, limited by the modest performance of the outdated Heusler crystal monochromator and the analyzer.

2. Beamline Productivity: 2

The instrument and instrument team does a very good job within the limits imposed by the instrument performance, and produce a well-balanced blend of elastic, inelastic and instrumentation productivity, whose quantity and quality are comparable to the other evaluated TAX instruments.

3. Leveraging of specific SNS/HFIR characteristics: 2.5

Due to its outdated PA infrastructure (Heusler polarizing crystals in particular) HB1 cannot adequately fulfil its PA role within the SNS/HFIR spectroscopy suite. Its current state resembles the pre-2000 configuration of IN20 at ILL.

4. Effectiveness of beam time use: 2

The instrument team makes efforts to use the available beam time as efficiently as possible. There are some complaints about scheduling of replacement experiments (discretionary beam-time) in cases of equipment failures, which tends to become more difficult due to the high levels of approvals currently required. This could be easily streamlined. At present, it risks some demoralization of the instrument scientists.

5. General User Program quality: 2

The user community demands and the breadth of the user program are fully consistent with those of the full TAX instrument suite. Greater direct feedback from the user community as to problems and satisfaction with all dimensions of the user experience (scheduling, technical support, sample environment etc) would be useful.

6. Adequacy and reliability of software, sample environment and ancillary equipment: 2

In contrast to the time-of-flight (TOF) instruments, the TAX software is not a bottleneck for productivity, but continued attention to its development and maintenance is needed. However, the shortage of technical personnel related to sample environment support and the low redundancy of the sophisticated sample environment leads to scheduling problems, loss of beamtime, and general inefficiencies associated with the productivity of the user program.

7. Future instrument science and development plan: 2.5

HB1 should play an important role as a polarized neutron complement to both the HB3 and the SNS thermal spectroscopy suite (ARCS, SEQUOIA). The instrument team states an ambition to bring polarized TAX to an internationally competitive level, however it is not currently clear that a development plan is in place that will allow this to occur in a timely fashion.

Our suggestions:

1. 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).

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

3. 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.

8. Overall Recommendation: Continuation

HB1A PhiTAX

This TAX instrument has rather constrained space, and it employs a double PG monochromator at a fixed energy, such that it utilizes a very clean Ei=14.7 meV incident beam, primarily for elastic scattering studies with good signal to noise. Both its user demand and its scientific productivity are high.

1. Scientific Mission and Impact: 2

HB1A is primarily a diffraction, or elastic scattering instrument for studies of structural transitions, magnetic order and phase transitions in a wide variety of single crystals as well as epitaxial thin films and multilayer materials. These measurements are carried out as a function of temperature, applied magnetic and electric fields, and pressure. It serves a large and broad user community.

2. Beamline Productivity: 2

The rate of publications on HB1A is very good, and it regularly contributes to a number of high impact publications.

3. Leveraging of specific SNS/HFIR characteristics: 1.5

HB1A plays an important role in the HFIR TAX suite of instruments, as it carries out an important program of elastic scattering measurements, and many parametric studies, and thus frees up the remaining TAX instruments to study primarily inelastic scattering. It has a high level of productivity. Given the space constraints at its position at HFIR, there is no easy comparison with similar instruments around the world.

4. Effectiveness of beam time use: 2

HB1A is well managed by its instrument scientists, but lacks a number of features that most modern instruments of similar capabilities possess. There is a real need to automate and modernize this instrument.

5. General User Program quality: 1.5

HB1A is mostly used for diffraction, and has quite a broad user base with a high oversubscription. The breadth of materials science carried out on it is very good, and the user base is also broad, drawn from both national labs and universities.

6. Adequacy and reliability of software: 2

The data acquisition software is good. The analysis software could be improved but is adequate for most needs on HB1A.

Adequacy and reliability of the sample environment: 2.5

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.

7. Future instrument science and development plan: 1.5

A development plan exists to automate and modernize both the sample and analyzer portion of the instrument. This includes motorized beam-size limiters, and sample enclosure to reduce radiation fields, to improve signal-to-noise, as well as to reduce crosstalk with other nearby instruments. This will also reduce personnel radiation exposures by reducing ambient fields and the required time spent in the instrument areas. 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.

8. Overall Recommendation – Continuation

HB3

1. Scientific Mission and Impact: 1

HB3 is the highest thermal flux TAX at ORNL. It is the workhorse instrument for inelastic studies under extreme conditions; high magnetic fields, high and low temperatures, as well as high pressure. The scientific impact of the instrument is excellent, *given the antiquated analyzer systems*. However, neutron scientists in the U.S. remain at a disadvantage compared to their European competitors and some forefront science is being missed.

2. Beamline Productivity: 2

The productivity of HB3 has been excellent, both in terms of number of publications and their impact.

3. Leveraging of specific SNS/HFIR characteristics: 2.5

Given the inherent very high flux available at the HB3, this instrument should be a best-in-class internationally. Presently this is not the case.

4. Effectiveness of beam time use: 2

The use of HB3 beamtime has been quite good. However, inadequate sample environment support has lowered the efficiency of operations for all the TAX spectrometers at HFIR, including HB3.

5. General User Program quality: 1

The breadth of the user science program at HB3 has been very good. The breadth of the community is also good with users drawn from both national laboratories and universities.

6. Adequacy and reliability of software, sample environment and ancillary equipment: 2

The data acquisition software is good. While the analysis software meets basic user needs, it could be improved.

Adequacy of sample environment support: 2.5

The level of sample environment support is inadequate. Backup sample environment equipment is often not available in the event of a sample environment failure. Inadequate support staff and infrastructure have resulted in losses of beam time.

7. Future instrument science and development plan

1. 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.

2. 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.

3. 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.

8. Overall Recommendation: Continuation

CTAX

CTAX is the only TAX at ORNL that looks at a cold source, although its cold neutron guide position is not optimal, and its flux is relatively low.

The observation of spin and atomic dynamics in the cold-neutron energy range quite often provides crucial information in condensed matter sciences. Hence, the necessity to have well designed cold-neutron inelastic instruments is clear. However, the current situation for CTAX is ambivalent. It is the only cold-neutron triple axis spectrometer, and it is needed; however, its low flux significantly limits its applications for cutting-edge sciences, and makes CTAX less than fully complementary with its SNS counterpart, CNCS. It should be noted that the instrument produces a reasonable amount of high-quality scientific output, nonetheless. However, if properly illuminated by high-flux neutrons, the cold-neutron triple-axis can do much more and should aspire to be competitive to the leading spectrometers in the world. Such a high intensity cold-neutron triple-axis spectroscopy will fill up the missing part of the HFIR/SNS instrument matrix, and will complete the three sources strategy of whole ORNL neutron program.

1. Scientific mission and impact
(Scientific mission: 1 – Impact: 3)

Cold neutron inelastic spectroscopy is a key capability of the neutron scattering technique, and the role of the cold-neutron triple-axis spectroscopy in, for example, quantum magnetism and correlated electron research, is very important.

The relatively low flux associated with the present CTAX position on the cold neutron guide limits scientific application, and hence, its impact is lower than it otherwise would be or should be.

2. Beamline productivity: 2

The productivity at CTAX is reasonably high over the last 4 years with 6 high-impact (IF>7) papers. This is viewed as quite good in light of the low incident flux at CTAX.

3. Leveraging of specific SNS/HFIR characteristics score: 3

Cold neutron inelastic spectroscopy is in very high demand over the full ORNL suite of inelastic instruments at SNS/HFIR. Presently CNCS is the only optimized, workhorse spectrometer for this energy range, and it is extraordinary oversubscribed. A large enhancement of the incident neutron flux is necessary for CTAX to be complementary with CNCS, and to give the SNS/HFIR instrument matrix full coverage.

4. Effectiveness of beam time use score: 2

With the exception of 2014, when the new doubly focusing analyzer was commissioned, CTAX beam time has been allocated and used effectively by the general users.

5. General user program quality score: 2.5

The incident neutron flux is a significant limiting factor in-so-far-as running a high-quality user program is concerned. Within the context of this limitation, the quality of the overall user program is high.

6. Adequacy and reliability of software, sample environment and ancillary equipment: 2.5

The SPICE software works well and is sufficient to run experiments. However the analysis software could be brought up to date with greater functionality.

As is the case with the rest of the TAX suite, sample environment issues have limited productivity due to an inability of the staff to respond to evening and weekend requests for support, and due to a lack of redundancy in specialized sample environment equipment.

7. Future instrument science and development plan: 1

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.

8. Overall Recommendation: Continuation

1. 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.

Instrument Reports – Time-of-Flight Direct Geometry Chopper Suite:

ARCS:

1. Scientific Mission and Impact: 1

ARCS is a direct geometry chopper spectrometer with a relatively short sample to detector distance (3 m) and large coverage of reciprocal space. This makes it ideally suited to the comprehensive studies of lattice vibrational spectroscopy. However, several fields of hard condensed matter research take advantage of ARCS, including magnetism and correlated electron physics. The publication record is quite good in many fields, and has been of high impact. For example, the fraction of "high impact" publications that ARCS produces is 30%, when those publications have an author from the NScD.

2. Beamline Productivity: 1.5

ARCS has been in a steady state of good productivity for several years now. With its present oversubscription rate of 3.5, which is too high, this will not likely change.

3. Leveraging of specific SNS/HFIR characteristics : 1

The instrument is well matched to the source, and will benefit directly from improvements in the power and performance of the target.

4. Effectiveness of beam time use: 1

ARCS produces about 2.5 experiments per publication, which is probably about as high as can be expected if new science (and high impact publications) are to be performed.

5. General User Program quality: 1

The scientific output is excellent, and unusually diverse for an instrument at the SNS.

6. Adequacy and reliability of software, sample environment and ancillary equipment: 2

The sample environment capabilities should be rated at 2. Overall, the sample environment capabilities for the direct geometry instruments have improved considerably. Challenges remain for high pressures and high magnetic fields, but this is expected.

The software capabilities should be rated lower. Again, the situation has improved enormously since the early days of the SNS, and software is always difficult because its demands and its capabilities are not so obvious.

The update of the data acquisition system of ARCS is essential. We hope that lessons learned in replacing data acquisition systems for other instruments will minimize the disruption of the installation and testing of the new system ARCS.

At a higher level of analysis, the software support for ARCS generally meets up with where users can take over. Analysis for powders is in good shape, but the single crystal software tools are in need of updating.

7. Future instrument science and development plan: 2

ARCS has had an update for its vacuum system, and is scheduled for an update in its data acquisition system. A multiple-sample changer for a cryostat is a good idea, and in the works. There is a good plan to understand how a disc chopper will offer new capabilities on ARCS, improving its energy resolution for medium incident energies and for dynamic PDF analyses. Perhaps it would be appropriate to consider the science impact of rep rate multiplication, as well.

8. Overall Recommendation: Continuation

ARCS is doing well, and its current staff have served its needs and user community well. It should be allowed to continue on its path.

Specific recommendations for improved performance are to:

1. Replace the data acquisition system.
2. Develop and deploy a multi-sample changer for samples at room temperature and below.
3. Complete an analysis of the benefit of a disc chopper for energy resolution improvements that could improve dynamical pair distribution function analysis.

SEQUOIA Chopper Spectrometer

1. Scientific Mission and Impact: 1.5

SEQOUIA is the best in class thermal chopper spectrometer with a relatively large sample to detector distance (5 m) and a corresponding focus on relatively low Q. As such it is very complementary to ARCS. Its closest international comparator is MAPS at ISIS. Its overall program is heavily magnetism-based, as intended by design.

The detector complement should be filled out to the extent possible. A radial collimator needs to be added so that large sample environment apparatus can be accommodated. Magnet design will also need to be carefully considered in order to produce useful in –magnetic field data on SEQUOIA.

2. Beamline Productivity: 1.5

The scientific productivity is approaching 1 publication for every 2 experiments run which will be hard to improve upon.

3. Leveraging of specific SNS/HFIR characteristics: 1.5

SEQUOIA is fulfilling its role as the world's leading fine resolution direct geometry chopper instrument. It is appropriately leveraging the SNS characteristics and its capabilities are not duplicated. It would leverage the SNS characteristics better if it were to fill out its complement of detectors and employ a high resolution chopper.

4. Effectiveness of beam time use: 2

SEQUOIA's beamtime appears to be used effectively. It is oversubscribed by a factor of 3.5, which is high. Given the pressure on the GU competition and the fact that the structure of the IDT has recently changed, it may be worthwhile to fully consider how the IDT time is used.

5. General User Program quality: **2**

The quality of the GU program appears to be high, as indicated by the rate of publications forthcoming, and their quality.

6. Adequacy and reliability of software, sample environment and ancillary equipment: 3

Sophisticated sample environment is lacking due to the high background caused by the lack of an effective radial collimator. Plans are in place to acquire an appropriate radial collimation, which will enable the use of magnet cryostats and perhaps high pressures. Given the emphasis on magnetism by design, this appears to be quite important.

As with all the chopper instruments, beamtime productivity is limited by data visualization and analysis capabilities, especially for single crystal studies.

7. Future instrument science and development plan: 2

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.
2- Filling out SEQUOIA's complement of position sensitive detectors thereby making SEQUOIA much more efficient.
3- The incorporation of a low angle detector bank to enable Brillouin scattering (relatively high energy transfers at low wavevector transfer).

The first two of these will clearly result in enhanced scientific capabilities and greater productivity. The third area for development, the low angle bank to enable Brillouin scattering, should be better developed with a science and business case detailing what will be gained at what cost.

8. Overall Recommendation: Continuation

CNCS

1. Scientific Mission and Impact: 1.0

CNCS is the premier cold neutron TOF spectrometer in the world. Its user base is hard matter centric, and it is already very heavily oversubscribed.

2. Beamline Productivity: 1.0

The beamline productivity is close to 1 publication for every 2 experiments run, which is hard to improve upon. At the same time, the instrument continues to push new measurements, especially with regard to sophisticated sample environment, such as high pressures.

3. Leveraging of specific SNS/HFIR characteristics: 1.0

CNCS plays a unique role in ORNL's suite of inelastic capabilities, and to that extent that it is badly oversubscribed. This will change with the development of cold neutron spectroscopic capabilities at the STS and with MANTA at HFIR, but these will not affect the user program for at least 5 years.

4. Effectiveness of beam time use: 1.5

Development of pressure capabilities using discretionary beamtime has been successful, and it is clearly of great interest and with potential for high impact.

5. General User Program quality: 1.5

The General User Program is of high quality, but the oversubscription rate for the instrument (~ 4 to 5) is very high. This is problematic, and potentially off putting, in that it is hard for the user community to plan appropriately with such a high oversubscription rate.

6. Adequacy and reliability of software, sample environment and ancillary equipment (software 2.5 – Sample Environment and ancillary equipment 2)

The recent change of the DAS brings many improvements for planning and performing single crystal experiments, although it is still in the early stages of implementation and needs further improvements. There had been many efforts over the years for improving data reduction and advanced algorithms are available within the Mantid framework. However, most users are not aware of these or do not know how to use them. For this reason, efforts are needed to provide a user-friendly data reduction workflow across all direct time-of-flight instruments. There is also the need for developments of tools for analyzing and visualizing four-dimensional S(Q,w) data sets.

Features that would greatly help users analyze their data (and hence accelerate publication) include convolution of instrumental resolution, either locally with simplified models for excitations (linear or quadratic) or globally with complex models for S(Q,w). It is felt that the availability of scientific software to analyze single-crystal TOF data would greatly increase the speed of publication, as well as to allow for new publications from observations in the measured data that would otherwise have been overlooked.

Sophisticated sample environment (magnet cryostats in particular) have been lacking in the past, although recent plans for acquisition are promising. In addition, such sample environments require radial collimation which is now being upgraded and installed. In the near future, we expect the suite of sample environments to be commensurate with the world's premiere cold TOF instrument. The sample environment group should be commended for the development of high pressure capabilities as this has the potential to bring exciting new science to this instrument.

7. Future instrument science and development plan 1.5

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.

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.

8. Overall Recommendation: Continuation

HYSPEC

1. Scientific mission and Impact: 2

The scientific brief of the instrument team is well founded and focused - i.e. the development of polarized neutron facilities for direct geometry spectroscopy (DGS). Some significant steps have been taken, and the instrument is clearly "finding its feet". HYSPEC is the only example of a polarized direct geometry chopper spectrometer (DGCS) at a pulsed source. Polarized neutron development work should continue to be strongly supported by SNS on this instrument.

It is a concern that the publication rate from the instrument is low and rather flat over the last three years. This is somewhat to be expected for an instrument focused on polarized neutron experiments, and for a new instrument - but the instrument team should attempt to identify what are the major barriers to increased publication.

2. Beamline productivity: 2.5

With low publication numbers and relatively few high impact papers, the output of HYPSEC is a concern (see above). However, we are convinced that HYSPEC is rather productive in the sense of its development of a DGCS with polarized neutron scattering, and we note that in this specialist area it is currently unique in the world. Post-doc experimental support might well be crucial in increasing productivity. The fostering of a wider user base will also help in this regard.

3. Leveraging of specific SNS/HFIR characteristics: 1

This instrument fulfils several important functions within the SNS and HFIR landscape. It is part of the strategically crucial and oversubscribed cold spectrometer suite. It is a trailblazer for polarized DGCS, and it is the latest in a long line of attempts to amalgamate pulsed and steady state source techniques. In some ways, it is the only truly unconventional inelastic instrument at the SNS. The massive neutron flux at the SNS and the relaxed resolution of HYSPEC are exactly what is required to make a successful DGS polarized instrument.

4. Effectiveness of beam time use: No ranking

This is difficult to judge, as considerable beamtime has been devoted to the development of polarization analysis capabilities, which is important, but which has not led to much productivity as of yet. It would be useful to see the breakdown of publications from internal vs BNL usage of the beamline. It would also be useful to see statistics on lost time - failed experiments, bad crystals, poor users, etc.

5. General User Program Quality: 2

This is also difficult to judge this. The oversubscription factor is healthy - so it is likely that the quality of the proposed experiments is high. Much will depend on the availability of high quality single crystal samples - since this instrument is unlikely to measure anything other than single crystals. The selection of publications presented by the instrument team shows data of high quality.

6. Adequacy and reliability of software, sample environment and ancillary equipment: 2

The provision of high magnetic field and concurrent low temperatures is vital to cold neutron spectroscopy. HYSPEC has access to a 5T asymmetric magnet, with options to use an 8T symmetric magnet (for half polarized studies), and possibly a new 14T magnet.

Software has emerged as a common deficit for DGS instruments. It is good to see a dedicated effort on polarization analysis data reduction. HYSPEC will benefit - as will all DGS machines - from further efforts on data modelling in the form of easy interfacing with third party codes (e.g. SpinW), and inclusion of the full instrument resolution model.

7. Future instrument science and development plan: 2

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.

They have specifically asked about whether they should include 3He 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.

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.

It is commendable that efforts are being pursued in the direction on Spherical Neutron Polarimetry, and half-polarised 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.

9. **Overall Recommendation: Continuation**

Our suggestions, in priority order:

1- increase efforts on software - data reduction and modelling with resolution
2- Investigate and understand the main barriers to publication from HYSPEC experiments
3- go ahead with the project to install analyser changer/oscillator
4- go ahead with the commissioning of z-only PA in field
5- launch a project to look at implementation of a secondary spectrometer wide-angle flipper.