ORNL/TM-2022/2509

Oak Ridge National Laboratory Second Target Station Instrument Systems Research and Development Plan

Leighton Coates
Anton Khaplanov
Van Graves
David Anderson
John Ankner

June 21, 2022

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Second Target Station (STS) Project

Second Target Station Instrument Systems Research and Development Plan

Prepared by: Leighton Coates, STS Instrument and Technology manager

Leighton Coates

Digitally signed by Leighton Coates
Date: 2022.07.20 10:03:19 -04'00'

Approved by: Kenneth Herwig, STS Technical Director

Kenneth Herwig

Digitally signed by Kenneth Herwig
Date: 2022.07.20 11:07:01 -04'00'

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1. LIST OF ABBREVIATIONS

AC	Anger Camera
ANSTO	Australian Centre for Neutron Scattering
BWAVES	Broadband Wide-Angle VElocity Selector
CPU	Central Processing Unit
FDM	Fused Deposition Modeling
FTS	First Target Station
FOM	Frame Overlap Mirror
GPU	Graphics Processing Unit
HV	High Voltage
ILL	Institut Laue- Langevin
JIT	Just In Time
LLB	Laboratoire Léon Brillouin
LDRD	Laboratory Directed Research and Development
LPSD	Linear Position Sensitive Detector
MC	Monte Carlo
MCP	Multi Channel Plate
MDF	Manufacturing Demonstration Facility
MT	Monoblock multi tube
NScD	Neutron Science Division
NTD	Neutron Technologies Division
ORNL	Oak Ridge National Laboratory
ROC	Read Out Channel
R&D	Research and Development
PCB	Printed Circuit Board
PLA	Polylactic Acid
PPU	Proton Power Upgrade
SiPM	Silicon Photo Multiplier
SLAC	Stanford Linear Accelerator Complex
SNS	Spallation Neutron Source
STS	Second Target Station

2. INTRODUCTION

This document describes the research and development (R&D) plan for Second Target Station (STS) instruments and bunker. The R&D program at STS seeks to mitigate risk and develop new technologies that will enhance performance for deployment on the eight instruments that are part of the STS project. Currently, STS is actively developing six of the eight instruments. This document is expected to be revised as the R&D program progresses and activities begin on the remaining two instruments (VERDI and EXPANSE).

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL), which began operating in April 2006, provides the United States with a world-leading source of pulsed neutrons for research. As currently configured, SNS delivers 60 Hz pulses of high-energy protons to a liquid mercury target, where bursts of neutrons are produced when protons collide with the nuclei of mercury atoms. This First Target Station (FTS) is optimized to produce thermal neutrons (i.e., neutrons with wavelength $\lambda \approx 1.8$ Å) at high wavelength-resolution that are ideal for spatial resolutions on the atomic scale and fast dynamics studies of materials.

The Second Target Station (STS) Project substantially expands the capabilities of SNS to meet global needs for a high-intensity source of cold (long-wavelength) neutrons and sustain US leadership in neutron scattering for decades to come. Planning for the STS began during the initial SNS project stage, and Critical Decision 1 (CD-1) was approved in November of 2020 for a facility with capabilities complementary to those of the FTS and optimized to produce cold neutrons. The Proton Power Upgrade (PPU) Project, initiated in FY 2018, will double the power of the SNS accelerator complex to 2.8 MW which will be used to increase proton power on target to 2 MW at FTS and provide 700 kW to STS. Every fourth pulse will be diverted to STS which will operate at 15 Hz while the remaining pulses are directed to FTS. The STS Project will provide researchers from a wide range of disciplines with a facility that offers wholly new experimental capabilities for addressing key questions across a range of scientific areas. An extensive instrument selection process was held between August 2020 to August 2021, with 12 instrument proposals being reviewed by an external committee of 22 scientists. This process concluded with the selection of the eight instruments that will be constructed as part of the STS. The instruments that will be built as part of the STS project are

BWAVES, a broadband wide-angle velocity selector spectrometer, will simultaneously probe dynamic processes spanning 4.5 orders of magnitude in energy transfer, measuring continuous spectra that comprise both vibrational and relaxational excitations, from 0.01 meV to hundreds of meV. It will enable neutron scattering studies of dynamics in materials over the broadest possible range, especially complex biological, soft, and chemical systems characterized by dynamic processes spanning a wide range of time.

CENTAUR, a small-/wide-angle scattering instrument, will be designed to provide best-in-class resolution, dynamic range, and unique spectroscopic capabilities. The instrument will fully leverage the STS source, state-of-the-art neutron optics, and detectors to deliver unprecedented capability that enables simultaneous study of a wide range of length scales with high resolution, measuring smaller samples, and making time-resolved investigations of evolving structures in a wide range of scientific areas, such as soft matter, biology, material, geology, and quantum condensed matter.

CHESS, a direct geometry neutron spectrometer, will be designed to detect and analyze weak signals intrinsic to small cross-sections (e.g., small mass, small magnetic moments, neutron-absorbing materials).

It will be optimized for enabling unprecedented characterization of spin liquids, quantum magnets, thermoelectric materials, battery materials, liquids, and soft matter.

CUPI2D, a time-of-flight imaging instrument, will be designed for imaging dynamic processes in natural and engineered materials. It will have a transformational impact on scientific studies such as energy storage and conversion (e.g., batteries, fuel cells), materials engineering (e.g., additive manufacturing, advanced superalloys), nuclear materials (e.g., novel fuel cladding and moderators), cementitious materials, biology and ecosystems, and medical/dental applications.

EXPANSE, a wide-angle neutron spin echo instrument, will measure slow dynamic processes (neV-μeV) across a wide range of materials, including soft matter, polymers, biological materials, liquids and glasses, energy materials, unconventional magnets, and quantum materials. It will incorporate wide-angle detector banks, providing approximately two orders of magnitude Q-range and a wide wavelength band providing approximately four orders of magnitude in Fourier times.

PIONEER, a high Q-resolution (maximum unit cell: 10^7 $Å^3$), single-crystal, polarized neutron diffractometer, will be capable of measuring very small crystals (i.e., x-ray diffraction size or ~0.001 mm^3), ultra-thin films (~10 nm thicknesses), and weak structural and magnetic transitions. It will significantly lower the sample size barrier for single-crystal neutron diffraction.

QIKR, a general-purpose, horizontal-sample-surface reflectometer, will be designed to exploit the increased brightness of the STS to collect specular and off-specular reflectivity data significantly faster than existing instruments. Delivering this brightness within a broad wavelength band will permit collecting complete specular reflectivity curves using a single instrument setting, enabling "cinematic" operation by which the user turns on the instrument and "films" the sample as it changes in the neutron beam.

VERDI, a versatile diffractometer, will have full polarization analysis capabilities for study of complex magnetic structures of powders and single crystals. The instrument will allow routine measurements of milligram-size samples, small-moment compounds, and diffuse signals. It will probe magnetic local and long-range ordering in quantum and functional materials that exhibit emergent properties arising from collective behavior.

The high brightness of STS cold neutrons enables study of smaller samples and time-resolved measurements, while its 15Hz repetition rate enables the use of broader neutron bandwidths. These key properties of STS enable new neutron scattering experiments to be conducted. Some of the instruments at STS, such as BWAVES, use novel components that require R&D to produce an article suitable for deployment at an operating neutron instrument. Existing detector technologies for reflectometry and imaging will need R&D to ensure they are compatible with the increased brightness and dynamic range the STS source provides.

Testing detector and beamline component prototypes with cold neutrons require sustained access to a pulsed source of cold neutrons at a development beamline. A cold neutron development beamline is unavailable at a pulsed neutron source within the United States. Therefore, STS will construct a temporary development beamline at the Spallation Neutron Source (SNS) located on beamline 14B that views a coupled cryogenic moderator, which is the closest match to the moderators that will be used at STS. The STS development beamline will allow us to test critical STS beamline components with neutrons up to 20 Ångstroms, enabling us to fully test detectors and beamline components before the construction of STS instruments begins.

3. GENERAL RESEARCH AND DEVELOPMENT AREAS

The following R&D areas contained with section 3 are generally applicable to multiple beamlines at STS. For example, supermirror analyzers will be used on the VERDI and EXPANSE instruments while additive manufactured components are likely to be used on all eight of the beamlines.

3.1 DEVELOPMENT AND TESTING OF SUPERMIRROR ANALYZERS

The EXPANSE and VERDI instruments at STS will heavily utilize polarized neutrons to address key scientific questions. VERDI will employ full polarization analysis to study increasingly complex magnetic materials, in which magnetic scattering features are often weak. These weak scattering features cannot be seen using the widely adopted strategy to separate magnetic scattering (using un- polarized neutrons) with temperature variation. A dedicated neutron polarization setup will be required for VERDI to address its key scientific driver to study magnetism. Neutron spin-echo methods deployed on EXPANSE require use of polarized neutrons to measure slow dynamic processes.

Both instruments feature large detector arrays, meaning that the scattered neutron polarization must be analyzed over a large area across a range of wavelengths. HYSPEC (Zaliznyak *et al.*, 2017) at SNS FTS uses a wide-angle polarizing super mirror array consisting of 960 supermirrors to cover a 60° arc (Figure 1).

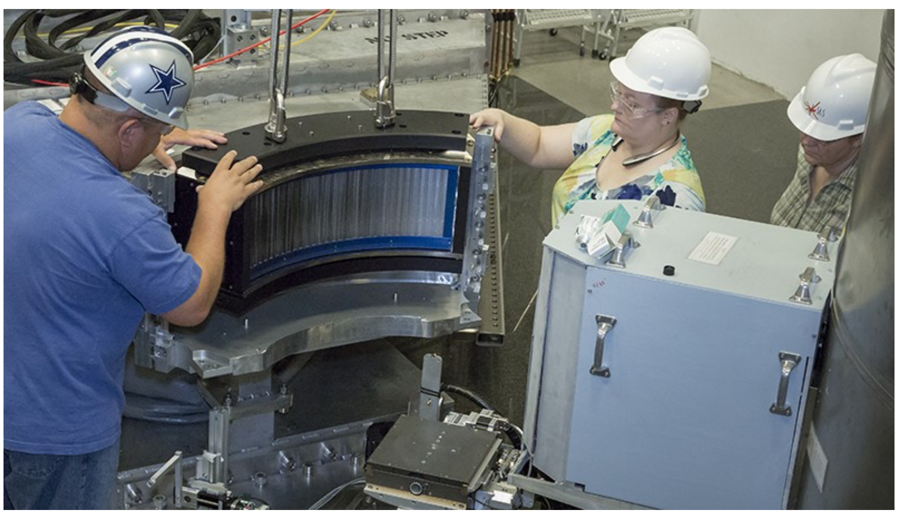

Figure 1: A wide-angle polarizing super mirror array at HYSPEC, SNS beamline 14B. The array consists of 960 supermirrors distributed in a 60-degree arc. Each mirror is covered in a multilayered coating of iron, cobalt, and vanadium alloys, allowing the mirrors to selectively reflect a specific neutron polarization state.

This requires the use of many supermirror polarization analyzers, presenting a challenge to the current capability and capacity of neutron guide vendors. To mitigate against this risk, we will work with US-based vendors to produce supermirror analyzers that we will test with neutrons at the Liquids Reflectometer (beamline 4B) at FTS (Ankner *et al.*, 2008). These tests will allow us to potentially develop new domestic suppliers and increase production options for the large number of polarizing supermirrors required by the VERDI and EXPANSE instruments.

3.2 ADDITIVE MANUFACTURING

Additive manufacturing or 3D printing has made a big impact in manufacturing by lowering costs and expediting production. This enabling technology also makes it possible to produce complex shapes that are impossible to create using conventional manufacturing methods. Collimators with highly complicated geometry can be quickly and easily manufactured by means of additive manufacturing (Figures 2 & 3), helping to increase the signal to noise ratio of neutron scattering experiments.

Figure 2: Small 3D printed neutron collimators have been used at the SNAP beamline at SNS to reduce background from small samples under high pressure.

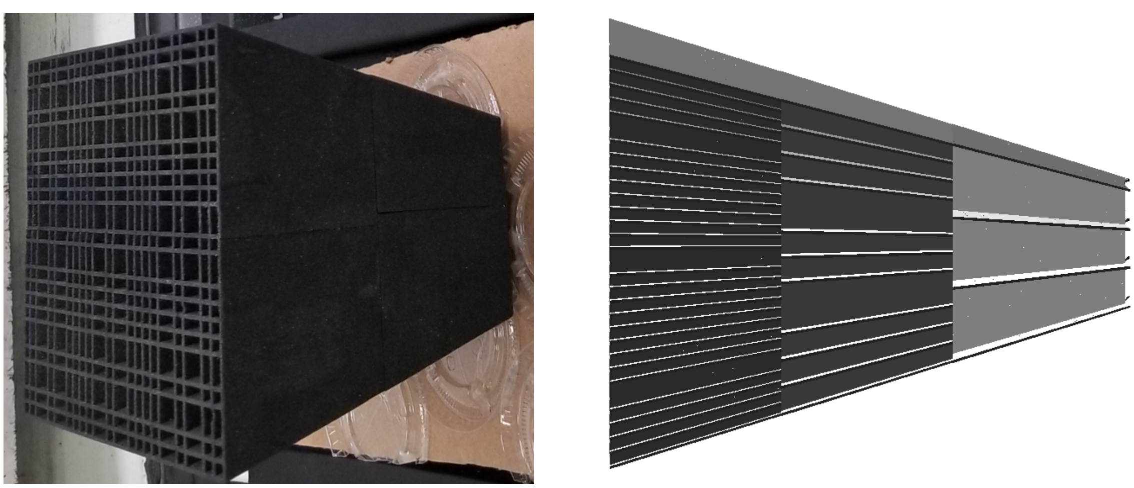

Figure 3: A complex, conical geometry collimator computationally designed from an algorithm written by Fahima Islam (Islam *et al.*, 2020). The left side shows the complete, printed device and the right shows a cross section. Additive Manufacturing is the only process that can be used to achieve this highly optimized geometry.

As an example, additive manufacturing provides the designer of a collimator the freedom to choose a geometry to favor a weakly scattering sample while suppressing Bragg peaks from a strongly scattering sample environment or other material which may be present on an instrument. The collimator in Figure 3 was designed exactly for this purpose (Islam *et al.*, 2020). Sample sizes at the STS will typically be an order of magnitude smaller than at SNS, requiring more complex collimators with finer features that would be difficult, impossible, or prohibitively expensive to manufacture using conventional methods. The Additive Manufacturing R&D effort will exploit technology developed by STS, NScD, and Manufacturing Demonstration Facility (MDF) researchers to 3D print collimators and other neutron scattering research instrumentation directly from neutron absorbing materials, typically Boron Carbide (B_4C) and enriched Boron Carbide ($^{10}B_4C$).

A 3D Printing Working Group has been established, which includes engineers and instrument scientists from the STS Project, as well as our main collaborator at the MDF, Amy Elliott. The group will identify new and existing methods to manufacture neutron absorbing apertures, collimators, and other devices by means of an additive manufacturing technique called binder jetting (see Figure 4) and develop new composite materials which include desired neutron absorbing characteristics.

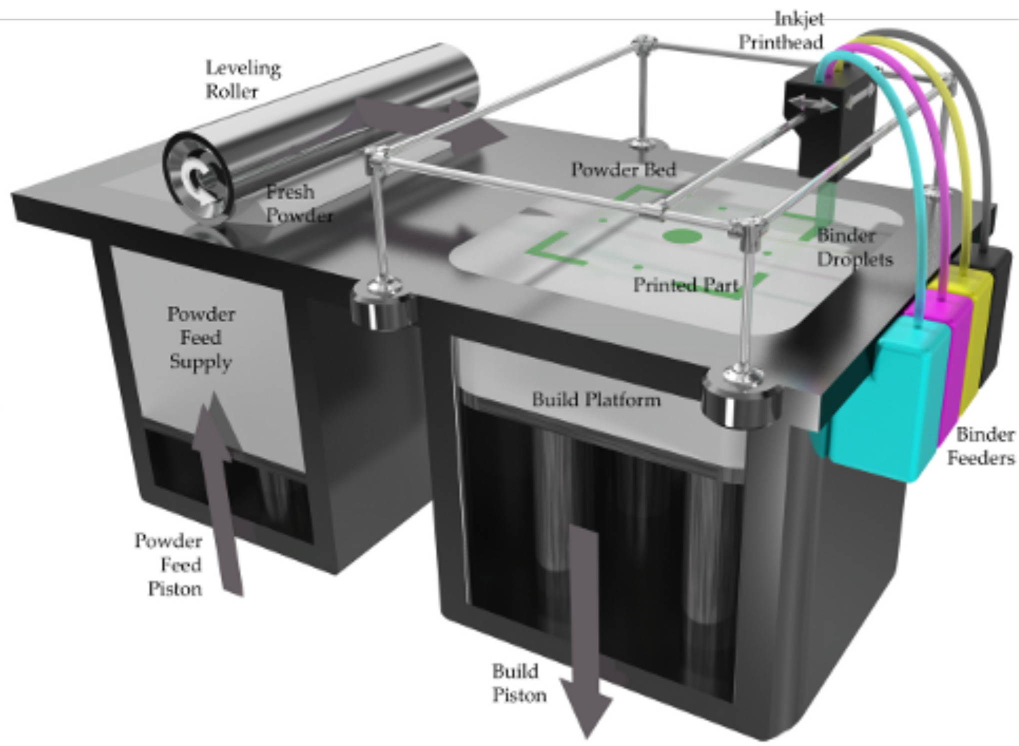

Figure 4: An illustration of a binder jet 3D printer, which uses a roller to spread a metal or ceramic powder from a feed supply to a build platform. An inkjet style printhead selectively deposits a binder, layer by layer, until a part is made.

Two popular applications of additively manufactured collimators, detector-mounted and sample-mounted, present very different challenges. A designer of a collimator that is mounted at the sample (or on a sample environment) typically wants to include features that are as small as possible, while a collimator mounted on a detector (or integral to the design of the detector) typically challenges the available build volume of a 3D printer. STS R&D activities will focus both on the finest level of detail that can reliably be printed as well as on manufacturing larger components. Additionally, attention will be given to eliminating alignment accuracy issues resulting from building larger assemblies from several smaller components, such as the collimator shown in Figure 3.

In FY22, to facilitate the prototyping of novel components, two 3D printers will be procured. The first will be a desktop FDM (Fused Deposition Modeling) printer capable of printing from standard Polylactic Acid (PLA) filament for test prints and concept development. The second printer will be a binder jet printer capable of printing boron carbide and other absorbing materials as shown in Figure 4.

3.3 MONOLITH OPTICS ALIGNMENT MOCKUP

To maximize the production of cold neutrons from a 700kW source, STS employs compact moderators tightly coupled to the neutron target, which means that STS neutron beams generally have much smaller cross sections than do the beams produced at the FTS. In addition, the average STS instrument length is 30% longer than the average FTS instrument. The combination of smaller beams and longer instruments results in higher precision alignment requirements of the neutron optics. The in-monolith optics of the STS also incorporate a different design than do their FTS counterparts, which results in monolith optic modules of ~4.5m in length.

Future instruments not installed during the project will require remote installation of their monolith optics, and the passive alignment scheme proposed for these optics is a significant risk to the project and to the future operation of the facility. To mitigate this risk, an R&D project is planned which will ensure that the optics which define the start of each beamline can be inserted into the monolith with the required alignment precision. To validate our monolith optic alignment design, we will construct a full-scale mockup of a section of the STS vacuum vessel with its extension nozzles that house the in-monolith optics (Figure 5). We will design full-scale mockups of the various in-monolith optic components (monolith inserts, optic modules, and monolith beam plugs) along with a prototypic handler designed to install each component for the initial eight instruments. This handler will be designed to install only "cold" (non-irradiated) components needed for the construction project; a separate "hot" handler will be developed later (when its design can be informed by experience with the cold handler) for future installations after start of operations that must be performed remotely.

There are several precursors to this R&D project taking place: mature preliminary designs of the monolith insert, the monolith insert beam plug, and the monolith insert optics module must all have been completed. Instrument Systems will produce the mockup designs of the inserts, optic modules, and beam stops in early FY 2023, along with the prototype handler and the mockup vessel components. Later in FY 2023, we will fabricate these components and the handler to create a mockup of the STS monolith. In FY 2024, we will conduct a thorough testing program with several cycles to identify any issues that could interfere with the remote insertion of the monolith optics. Results and lessons learned from this testing will be incorporated into the final designs of all the mockup components.

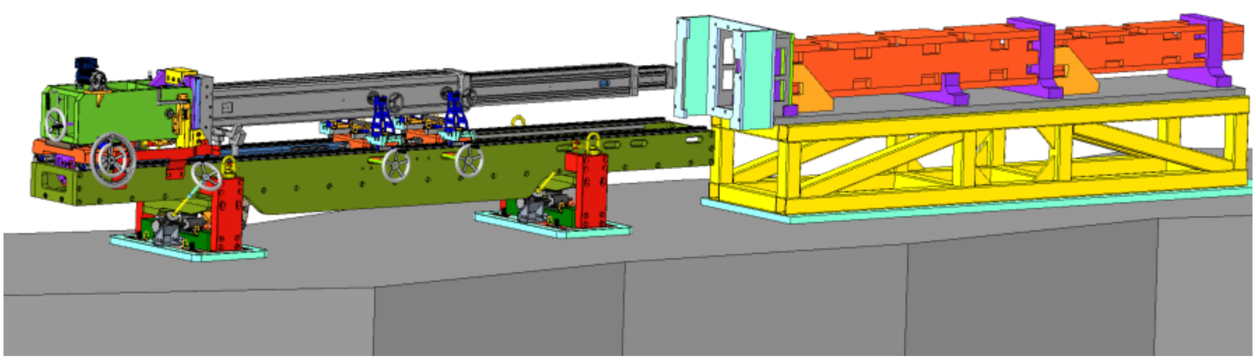

Figure 5: Monolith optics alignment mockup. The green cold handler is shown preparing to install the 4.5m-long grey monolith insert into the orange vacuum vessel nozzle extension, passing through the cyan shutter channel.

3.4 STEERABLE OPTICS MOCKUP

Several neutron scattering instrument concepts for STS incorporate advanced neutron optic designs which incorporate discrete mirrors rather than continuous neutron guides that were the standard for instruments in the First Target Station. These mirrors can be a few to several meters long and must be stably supported and aligned as a single optic. In addition, due to the length of the STS instruments and the small size of the STS neutron beams, installation and alignment at the micron level of precision will be required, which is beyond the ability of today's survey & alignment technology. Thus, a means of remotely adjusting these mirrors with single-digit micron resolution is needed. A Steerable Optic System mockup (Figure 6) has been designed to provide the precision and resolution required to support and manipulate these large, heavy optics under beamline shielding. This system is based on the original "magnet movers" developed at the Stanford Linear Accelerator Complex (SLAC) in the mid-90s and incorporated at synchrotrons worldwide. It uses eccentrically-mounted, motor-driven bearings with high-ratio gear reducers to orient and position objects in five degrees of freedom.

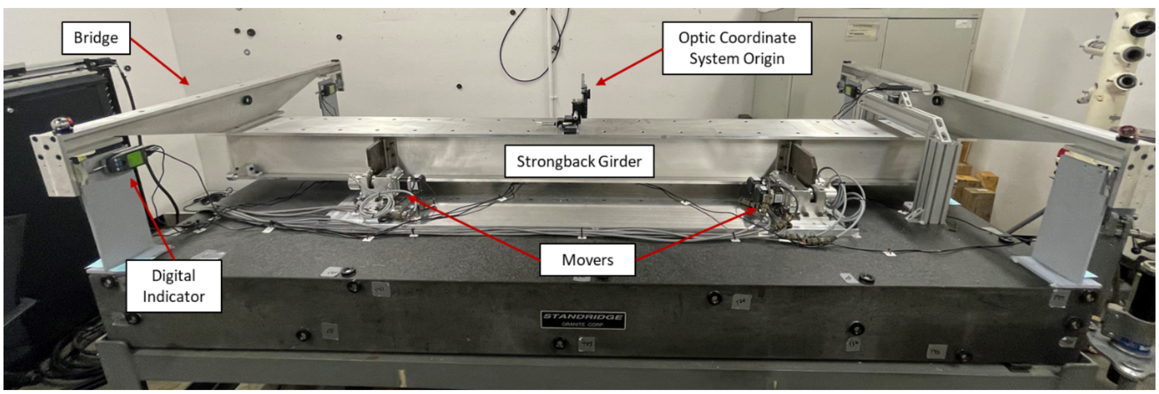

Figure 6: An image of the steerable optic mockup with key components labeled.

The steerable optics mockup system has undergone extensive testing and characterization studies. A full report of those tests and the detailed design of the steerable optics are documented in the steerable optics design and testing report (S07040200-TRT10000). In FY2023, we aim to complete our testing of the steerable optics design with neutrons at HFIR using a compact neutron optic and a high-resolution neutron camera.

3.5 GRAPHICS PROCESSING UNIT MONTE CARLO RAY-TRACING SIMULATIONS

Virtual neutron experiments using Monte Carlo (MC) neutron ray-tracing simulations by the MCViNE software package (Lin *et al.*, 2019) (Lin *et al.*, 2016) have proven useful in advanced neutron data analysis as well as instrument and sample environment design, including the initial design of the CHESS, and QIKR instruments for STS. Such simulations are also key to the accurate determination of resolution functions of neutron instruments, hence useful for super-resolution neutron data analysis techniques. The current MCViNE implementation makes use of the central processing unit (CPU) only. Graphics processing unit (GPU) computation has become an accelerator to many computation-intensive scientific applications. A Monte Carlo (MC) neutron ray-tracing simulation involves tracking many neutrons along their paths in a neutron instrument, and the parallelization of MC simulations is straightforward. Speeding up MCViNE with GPUs will make it more efficient and hence easier for STS instrument scientists to design new instruments and explore/validate more design options for STS and to be a useful future tool for users to plan and model experiments. In this project, for building up the GPU capability for MCViNE, we will use numba, an open-source JIT (just in time) compiler. Numba supports a subset of python and numpy code, and it allows developers to write python code but run it with performance close to machine code for both CPU and GPU. Based on experience with the McStas Monte Carlo ray-tracing package, speedups of two orders of magnitude are easily obtainable. The ability to conduct simulations more quickly allows us to explore more possibilities for neutron transport systems and to conduct more realistic virtual experiments. The ability of conduct realistic virtual experiments producing synthetic data will help to test software for data reduction before first neutrons will decrease commissioning time and help to ensure a productive early science program at the STS. This R&D effort will deliver a GPU compatible version of MCViNE by the end of FY 23 that will be used for advanced simulations of STS instruments and future instrument concepts.

4. DETECTOR R&D EFFORTS

Recently, an STS detector white paper (S04000000-TRT10000) was issued that defines the detector requirements and needed improvements to meet requirements for the eight STS project instruments. The detector R&D topics are designed to mitigate the risk of not reaching the required performance and thus not fully utilizing the increased brightness of the STS. Further, each development described below will achieve higher performance than currently available detector options.

4.1 HIGH-RATE DETECTORS FOR REFLECTOMETRY

Detectors for reflectometry require a combination of a high spatial resolution and high local rate capability. While an Anger camera fulfills the resolution requirement, a better rate capability can be achieved by a camera capable of reading out silicon photomultipliers (SiPM) sensor pixels individually. Prototypes of such a pixelated camera (Figure 7) have been successfully tested. However, more R&D is required to fully design and validate a suitable camera for a reflectometer at the STS.

For QIKR, a detector of this type would represent an improvement of 2-3 orders of magnitude in manageable neutron detection rate compared to currently available He3-based detectors used at FTS. This improvement will greatly enhance the capability of the instrument, allowing for samples with high reflectivity as well as for measurement of the direct beam with no attenuation – a crucial capability that currently does not exist on any reflectometer. A current limitation of a scintillator-based camera compared to a He3 detector is greater sensitivity to gamma rays. The R&D program will optimize the scintillator parameters to reduce gamma sensitivity as well as investigate the impact of gamma-ray and fast neutron background on the quality of reflectivity measurements. A combination of a reduced gamma sensitivity with appropriate background reduction measures in the vicinity of the detector is expected to produce acceptable signal-to-background while benefiting from a greatly increased counting rate capability. The R&D program for this new reflectometer detector will require test and validation measurements on a reflectometer beamline, such as the liquids reflectometer at SNS, as well as the STS Development Beamline, design and construction of prototypes, purchase of scintillators, SiPMs, and readout electronics. Further, a data acquisition system capable of storing and processing up to millons of neutron events per second will be required.

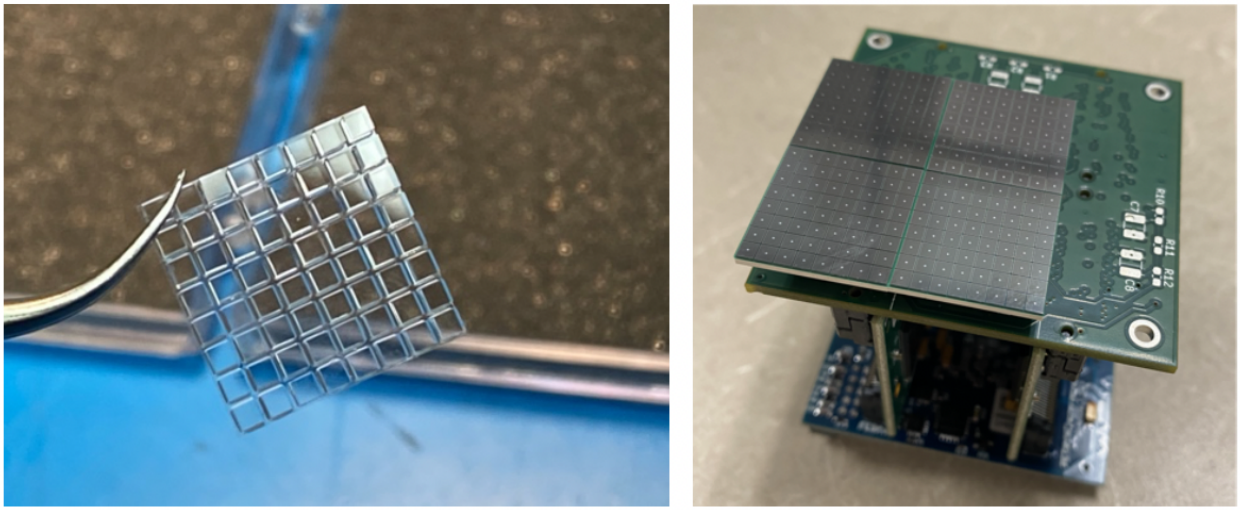

Figure 7: Pixel camera components. Left: segmented GS20 scintillator with 2-mm pixels. Right: Hamamatsu SiPM array with a 2mm pixel pitch designed to connect to the PETsys readout system.

The count rate performance of the SiPM pixel camera appears relatively certain. More unknown are the efforts needed to achieve the necessary sensitive area, increase position resolution to 1 mm and decrease gamma-sensitivity. Other scintillator options may be considered (Richards *et al.*, 2021) (Sykora *et al.*, 2018) in case of issues with pixelization of 1 mm, and if the required gamma insensitivity cannot be reached with GS20, a scintillator currently used on FTS Anger Camera detectors. The new pixel detector will not only fulfill the requirements of the STS reflectometers but will benefit reflectometers at FTS and essentially all other modern neutron sources. As a detector based on a concept from medical imaging, where vast fluxes of photons are used, the pixel detector promises to essentially solve the rate limitation in reflectometry. It does so while maintaining high detection efficiency and position resolution. Other instrument types may also benefit from the development, for example, SANS or diffraction with high expected rates.

4.2 VACUUM COMPATIBLE ANGER CAMERAS

Anger cameras (ACs) offer a combination of high position resolution and efficiency, making them suitable for many types of diffraction instruments. However, all instruments to date have ACs in air. On CENTAUR, the neutron flight path will be in vacuum, which means that a pressure-rated window would need to be placed in front of the cameras. The use of such a window would significantly attenuate longer wavelength neutrons negatively impacting the performance of the CENTAUR instrument. This R&D effort aims to design and validate the Anger camera for operation in vacuum. Reducing the risk of complications being found after construction that effect the performance of CENTAUR.

The current AC module will be separated into a front-end section (Figure 8), comprising the optical package and the preamplifiers, and a back-end section comprising the digitizers and the readout. Placing ACs in vacuum results in several complications. The optical package, including the sensor, diffusor, scintillator, and reflector need to remain stable and not delaminate under vacuum. The preamplifiers' heat output must be dissipated, and it needs to be verified that a stable temperature of the SiPM can be maintained. The detector needs to be galvanically decoupled from the vacuum vessel. Finally, the signals must be fed through the vacuum vessel in a way that does not induce noise.

The above challenges will be addressed in two R&D stages. The first stage is a proof-of-principle. Here, the individual components of the AC will be tested in vacuum with respect to heat dissipation. An operating AC will then be assembled where the front-end is in vacuum, and the back-end is in air. The two will be connected using vacuum electrical feed-throughs. In the second stage, a prototype detector module for CENTAUR will be built. This module must demonstrate the solutions derived in the first stage, the interface between neighbor cameras, and a prototype vacuum flange integration. Both the test detector from stage 1 and the prototype from stage 2 need to be tested in a neutron beam while operating under vacuum. For this, a dedicated vacuum chamber needs to be built.

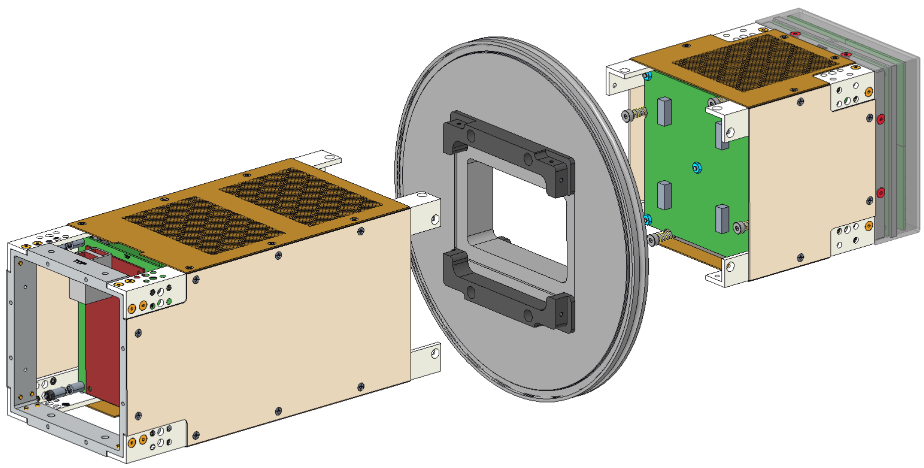

Figure 8: Engineering concept for a split Anger camera and flange. The neutron detector is on the right and would be in vacuum, while the readout electronics on the left containing the ROC boards would be in ambient air. The grey flange serves as the vacuum boundary.

The optical package – the scintillator and SiPM assembly – must be in a light-tight enclosure. Yet, this enclosure must be able to rapidly vent to vacuum during pump-down and fill with air during venting of the vacuum vessel. Failing this, the optical package would be (de)pressurized, causing stress or damage to the SiPM and movement of the scintillator with respect to the SiPM. During FY22 and early FY23 we will design and procure a dedicated vacuum chamber and complete testing with neutrons by the end of FY23.

4.3 HIGH-RESOLUTION ANGER CAMERA

As an additional capability, CENTAUR will be able to measure Spin-Echo Modulated SANS (SEMSANS). For this, a detector with a small area but a high spatial resolution of 200um or less is required in the direct line of the beam at the position of the small-angle detector. Few instruments in the world have this capability, making CENTAUR an instrument with a unique niche.

While the current generation of Anger Cameras based on GS20 Li-glass scintillator and SiPM readout can reach the resolution of 0.5 mm, an improvement in the scintillator light yield is needed to enhance resolution further. Several scintillators with a light yield higher than GS20 are known or are in development currently, although most have other drawbacks. Using one of these options, the performance needed for SEMSANS can be reached. An additional benefit of using an Anger camera for this high-resolution application is the use of only one type of detector throughout the whole detector array on

CENTAUR, mitigating the risk of poor results due to stitching of data of different formats collected by different detector types. We are currently working with several groups to identify promising new scintillator candidates that we can characterize and test to produce a high-resolution Anger camera. This R&D effort is envisioned to start in FY24 and will make use of the best scintillator candidates identified.

4.4 MULTI-TUBE MONOBLOCK DETECTORS FOR BWAVES

The Multi-Tube (MT) detector technology is an advanced form of He3 LPSD technology. Unlike conventional detector arrays built up from many individual tubes, the MT combines the necessary number of tubes into a monolithic detector body. The individual tubes are machined through the body and can thus be created in a variety of shapes and arrangements. As such, a tighter coverage can be achieved using tubes with a rectangular cross section, resulting in better uniformity and efficiency compared to a conventional row of round tubes. Multi-Tube technology (Abuel *et al.*, 2021) has been extensively used at the ILL, LLB, and ANSTO on eight instruments with 50+ total years of operation so far, demonstrating good reliability of the detector (Figure 10).

The Multi-Tube detector will greatly benefit the performance of BWAVES. The BWAVES instrument (Mamontov *et al.*, 2022) has a highly innovative design. To achieve the required performance, BWAVES has a short incident neutron flight path, with the detector located as close as possible to the bunker wall. The energy resolution of the instrument is limited by, among others, the detector depth contribution to the Time-of-Flight (ToF) resolution. For a tube of 8-mm diameter, the detector sets a limit on the instrument resolution of about 5.5%. This value is not acceptable as there is a risk that many experiments cannot be done with the needed resolution. The MT offers a way to reduce the detector depth to 4mm and possibly less. The resulting 2.75% contribution to the instrument energy resolution is comparable to other resolution terms, and the detector is no longer the limiting component. Additionally, the MT allows the detector area to be tiled more evenly, using rectangular tubes and only a single inter-tube wall.

The R&D into the MT technology will enable the design, delivery, commissioning, and operation of the final MT detector. An MT prototype will need to be built with tube dimensions similar to those of the final detector but only including a fraction coverage (~15%). Tubes with a 4mm cross section have previously been successfully used in the MT design. In order to further enhance the energy resolution of BWAVES, tubes with smaller dimensions will be investigated. Several different tube dimensions can be machined into the single MT prototype, thereby allowing a seamless comparison of performance as a function of tube dimensions.

The MT prototype will further enable the testing of the initial design of the BWAVES detector/rotor vacuum chamber. This vacuum chamber will be placed in a constrained space and will have to accommodate the detector and several other components. These solutions must be prototyped, including the integration of radial collimator, locations of signal feed-throughs, design of shielding, vibration mitigation, grounding, and more. A concept of the detector and WAVES rotor vessel based on a Multi-Tube detector is illustrated in Figure 9. The inner part (in black) is the WAVES device with the rotor at the top and the motor at the bottom.

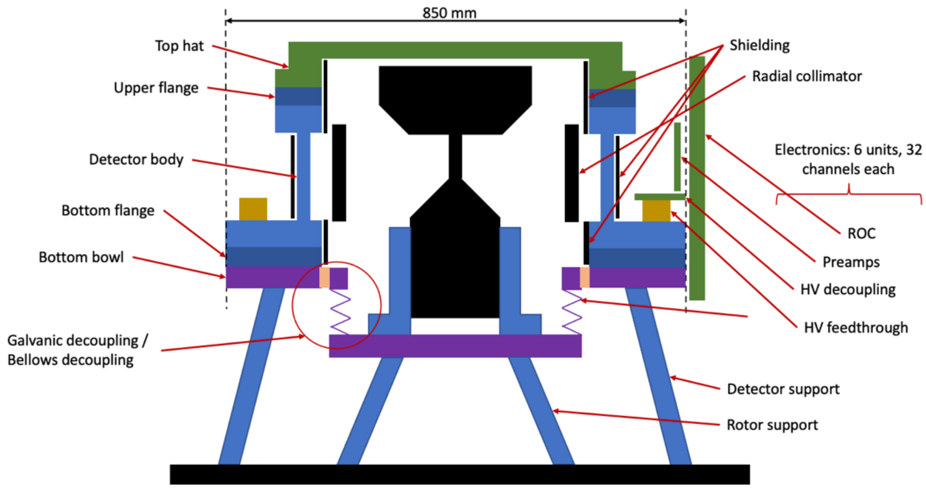

Figure 9: A concept of the detector and WAVES rotor vessel based on a Multi-Tube detector. The inner part (in black) is the WAVES device with the rotor at the top and the motor at the bottom.

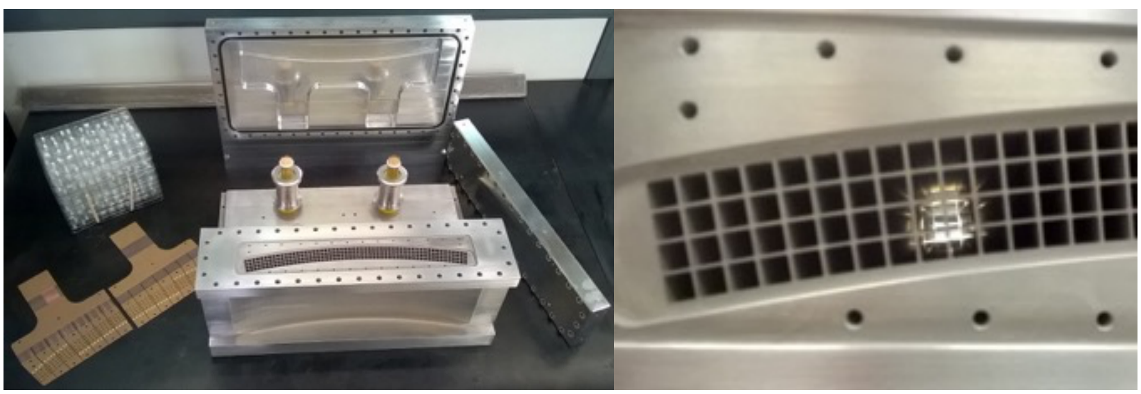

Figure 10: A curved Multi-Tube detector from the D3 instrument at the ILL. Left: the detector body and flanges. Right: closeup of the He^3 tubes machined through the aluminum block.

We will work closely with the detector group at ILL to design, procure and test a 120° monoblock wedge of a 600mm diameter circular detector that will enclose the WAVES rotor (FY 22-23). This monoblock wedge will be tested and characterized with neutrons in FY24 to complete this R&D activity.

4.5 HIGH RESOLUTION DETECTORS FOR NEUTRON IMAGING

A time-resolved neutron imaging detector presents a challenge in both the highest rate capability and the highest position resolution of any neutron detector type. Currently, the best time-resolved measurements have been obtained using a Timepix3-readout neutron-sensitive MCP detector (Watanabe *et al.*, 2017). Both the area of the Timepix and the area of the MCP set a limit of about 30x30mm^2 on the detector area achieved to date. The CUPI2D instrument requires an area of 100x100mm^2 with a count rate that exceeds the capability of the single-hit mode readout of Timepix3. Fortunately, the Timepix4 chip has now been made available for R&D within the Timepix collaboration. This new iteration improves on the predecessor by almost doubling the sensitive area, increasing the rate capability by an order of magnitude, and through the use of the through-vias, which allow the sensor to be joined to a printed circuit board (PCB) with no sensitive area.

A considerable R&D effort is required in order to achieve the requirements of the CUPI2D beamline. Two parallel efforts are planned. The development validation of an MCP neutron converter with larger than previously tested dimensions can be decoupled from the Timepix4 R&D in the first stage. Detectors with a large MCP area will be built using the proven Timepix3 readout (Figure 11). While this will not allow large images to be collected, it will help characterize and validate the larger MCPs. This development further mitigates risk in the quality of future MCPs. The supplier that had produced all neutron-sensitive MCPs up until now has ceased production and transferred technology to another company. Further, there is a risk in the uniformity of the MCP response over its area.

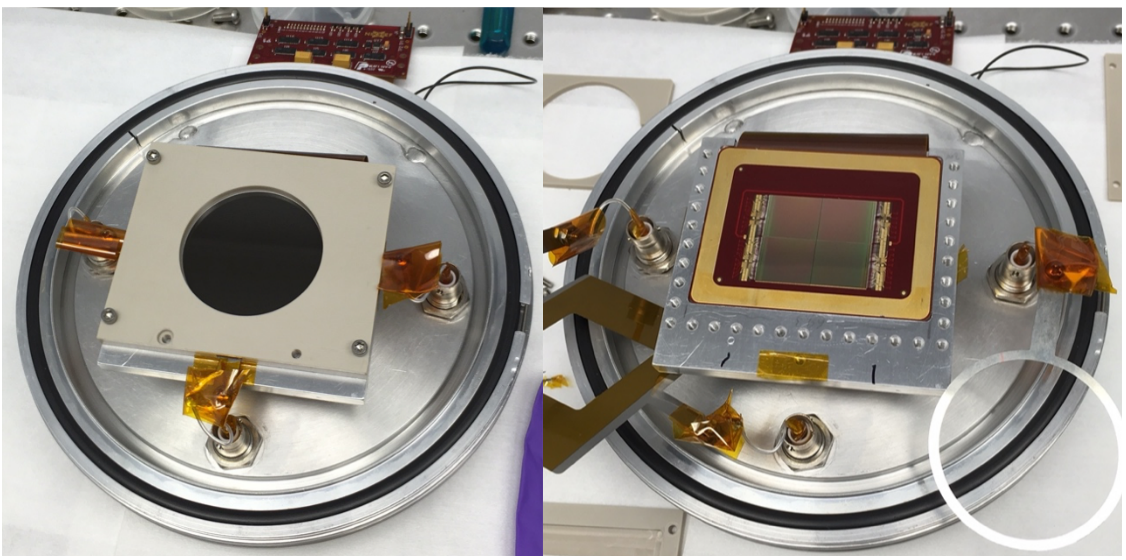

Figure 11: Components of a prototype imaging detector in their vacuum chamber. Right: a 2x2 array of Timepix3 chips. Left: Multi-channel plate (MCP).

The second R&D branch aims to develop the Timepix4 readout and integration and to efficiently process its data. This will enhance the performance of the existing Timepix3 systems and ensure that the required rate capability can be reached. The Timepix4 chip needs to be bonded to PCB, readout, the data processing pipeline established, and the neutron events reconstructed. The initial testing can be done with proven MCPs that are currently used in the Timepix3 systems. At the second stage of the R&D, the two branches will be merged in a detector that both uses the large-area MCP, as well as an array of 2x2 Timepix4 chips. This detector will have a sensitive area of 56x48mm^2. While only a quarter of the size of the detector needed for CUPI2D, it will demonstrate all technological and performance capabilities needed to build the final detector. We are currently working with commercial vendors to define a path forward for these R&D activities.

4.6 NEUTRON BEAM MONITORS

Beam monitors currently used at the FTS and in many other facilities do not have the dynamic range to accommodate the STS beams. A combination of several technologies is expected to fulfill the requirements for beam monitoring and thereby reduce the risks in commissioning, troubleshooting, and operation of instruments. Commercially produced monitors are expected to be used. However, R&D is needed to understand and validate their performance and, where insufficient, enhance performance.

Fiber monitors are highly attractive as a diagnostic monitor that has almost no impact on the beam and beam optics. It can also be translated in and out of the beam to minimize radiation damage. Even for a fiber monitor that can be translated out of the beam, R&D is needed to test and verify the radiation hardness of the scintillator and fiber. Additionally, a study of the sensitivity to gamma and fast neutron is needed. Silicon double-sided strip detectors have been recently proposed as a beam monitor for neutron beams (Cosentino *et al.*, 2015). While this is a well-known technology in charged particle detection, it has not yet been used for thermal neutron detection. An R&D project is currently underway at NTD, and an evaluation of the performance will be required for application at STS. We will closely monitor the R&D being conducted in NTD and develop our R&D plan to reflect the knowledge gained.

Multi-Tube monitors have recently been developed and successfully used at the ILL. This type of monitor has all the advantages of the He3 chamber – i.e., very low gamma sensitivity – while greatly increasing the rate and dynamic range capability. This monitor is likely to be suitable as a fixed beam integrating option.

5. STS DEVELOPMENT BEAMLINE

Several of the detector prototypes and beamline components detailed in the R&D plan will require extensive testing with time-of-flight cold neutron wavelengths of up to 20 Å. Currently, no such facility exists within the United States to conduct such testing. Therefore, STS will construct a temporary development beamline at the SNS FTS on Beamline 14B. The coupled hydrogen moderator on beamline 14 at SNS is a close match to the moderators that will be used at STS. This beamline is currently unoccupied and is expected to be available for use by STS personnel for a fixed period of time. In keeping with its temporary nature, the STS development beamline is designed to be easily removable, allowing for the future deployment of another beamline in the future.

The instrument design teams for the Spallation Neutron Source (SNS) Second Target Station (STS) propose to deploy innovative technologies to best exploit STS capabilities. The most ambitious of these ideas require an iterative process of development, testing, and refinement. To facilitate this work, we propose to construct a development beamline at the SNS First Target Station (FTS).

The unprecedented brilliance and wavelength bandwidth at STS pose challenges for present-day neutron detectors. Improvements in existing detector designs as well as the evaluation of promising prototypes will be required to optimize such characteristics as:

- Detection efficiency vs. wavelength
- Crosstalk in ^{3}He tube and scintillator arrays
- Pixel edge effects
- Time-of-flight performance
- High count-rate capability

- Beam monitors and cameras

A development station delivering pulsed thermal and cold neutrons will provide an environment as close as possible to the STS and enable testing under realistic conditions. Innovative beamline components such as focusing optics will be deployed at STS to transport the high brilliance delivered by its small neutron moderators onto small samples. Testing prototypes and eventually acceptance testing delivered components will be needed to ensure the successful deployment of such devices as

- Montel and other focusing optics
- Wide-wavelength-band spin polarizers
- Quality assurance and alignment of guide subassemblies
- Transmission of 3D-printed shielding and window materials
- Servo mechanisms for optics and sample alignment

Most of the instruments approved for the first round of construction at STS are refinements and/or extensions of existing instrument types. By contrast, the BWAVES instrument represents an entirely new type of instrument promising to offer unique performance over a broad range of scientific fields. The installation of a high frequency rotor near the sample and detector array will benefit enormously from the development and improvement cycle afforded by a dedicated development beamline.

To accommodate the needs outlined above, we have assembled a base requirements list:

- An open and accessible sample/detector space
    - Room to mount 2-m-long ^{3}He tube 8-packs: 3×1 m^2 transverse to and along beam
    - Room for several meter long focusing assemblies
- Platform/table
    - 1000 kg weight capacity
    - Configurable mounting scheme for user-supplied gear
    - Area ≥ 1×2 m^2 transverse to and along beam
- Full SNS FTS Data Acquisition System (DAS)
- Thermal and cold neutrons: 2 Å < λ < 20 Å
- Adjustable beam sizes and collimations
- Gap or gaps upstream to install beam monitors

5.1 STS DEVELOPMENT BEAMLINE CONCEPT

There is currently an unused port on beamline 14A (BL-14A) at the FTS. To satisfy the requirements in the available space at a reasonable cost we propose a design consisting of a disk chopper and three mirrors, shown schematically in Figure 12. Mirror 1 is set at a fixed shallow angle to the incident beam to reflect neutrons with λ > 2 Å. Shorter-wavelength neutrons pass through Mirror 1 and are absorbed in the beamstop. The Chopper cuts the reflected beam at 60 Hz and delivers 2-Å-wide bands of neutrons to the end station gated to the proton pulse on target. A single disk chopper periodically opens to pass unwanted neutrons generated by proton pulses before and after the chosen pulse, so a frame-overlap mirror (FOM) and a second reflection mirror (Mirror 2) serve as low- and high-pass wavelength filters, respectively, to reject these unwanted neutron bands.

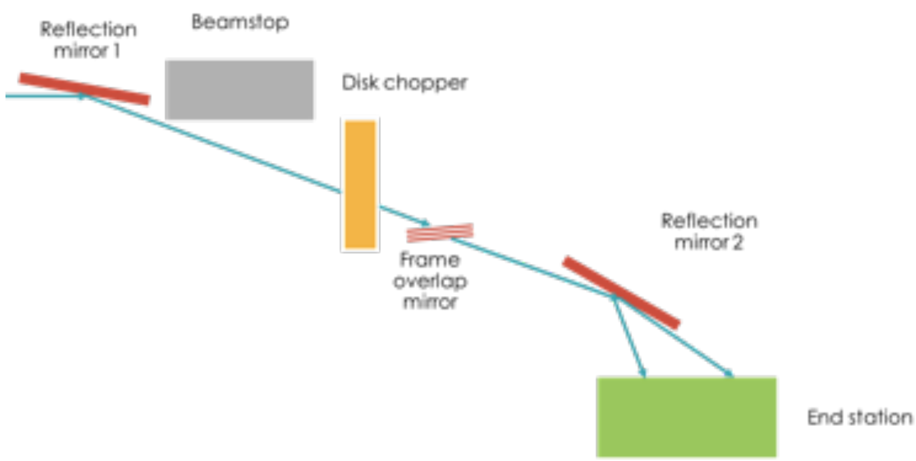

Figure 12: Schematic concept for the STS development station.

Figure 13 plots the transmission function of these components for a 2×2 cm^2 beam delivered to the end station 25 m from the moderator with the chopper phased to deliver a wavelength band centered on λ_c = 19 Å. The FOM is set at an angle of 110 mradian relative to the incident beam, reflecting out all neutrons with $\lambda > 21$ Å. Downstream of the FOM the beam passes onto Mirror 2, which is set to reflect all neutrons with $\lambda > 16$ Å into the end station. By this means we deliver a clean 2-Å-wide band (18 Å < λ < 20 Å) of neutrons. Different bands may be selected by rephasing the chopper and adjusting the tilt angles of the FOM and Mirror 2.

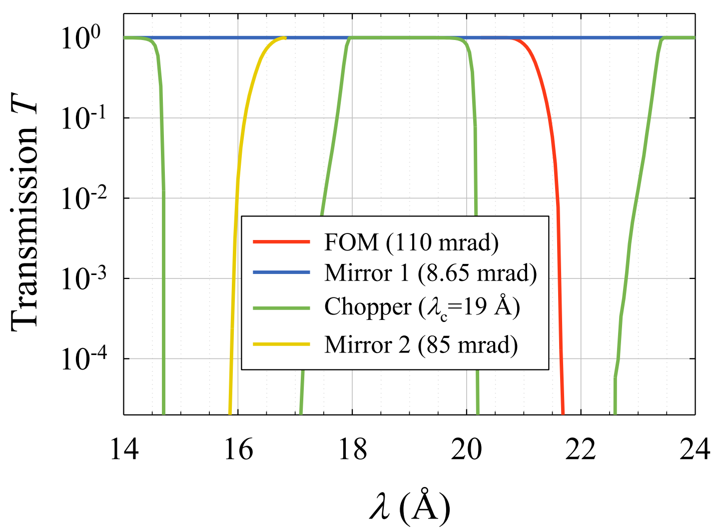

Figure 13: Transmission functions for beamline components set to deliver neutrons in a band centered on 19 Å.

An engineering drawing illustrating the proposed location of development beamline components within the existing available space at FTS BL-14A is shown in Figure 14. The components are arranged as shown in Figure 12, with the trajectories of the shortest (2 Å) and longest (20 Å) wavelength beams highlighted in blue and red, respectively. The sample area will be enclosed in a steel and concrete bunker.

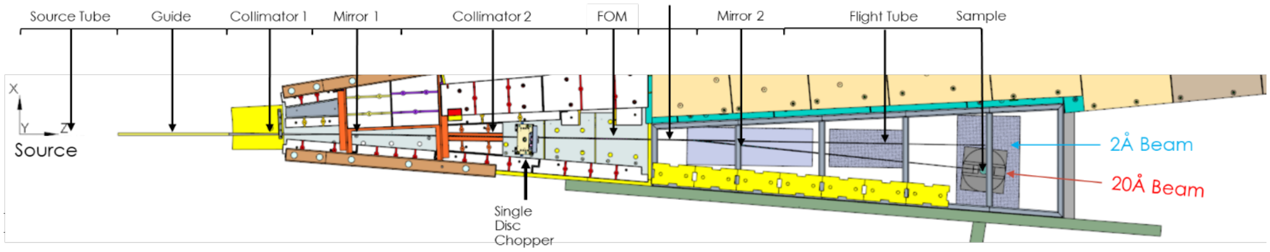

Figure 14: Component layout in available space at FTS BL-14A.

Acceptance diagram and chopper transmission simulations have been employed to calculate the intensity of neutrons from the FTS moderator delivered through a 2×2 cm^2 beam tube onto Mirror 2 (Figure 15).

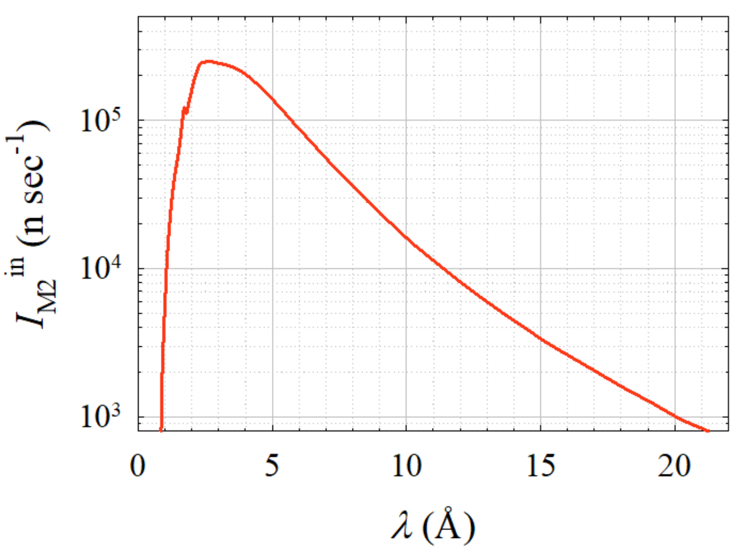

Figure 15: Neutron count rate delivered from the FTS BD moderator via upstream optics in a 2x2 cm^2 beam tube onto mirror 2.

Two *x-y* slits downstream of Mirror 2 will select the desired beam size and angular divergence into the sample area. A floor-spanning breadboard platform will be provided for users to erect support structures for the objects under study in their experiments. Currently, we are finalizing a cost estimate for design and construction of the STS development beamline. With a provisional plan to submit a beamline request proposal to NScD in the summer of FY22. With beamline installation occurring between September 2023 to September 2024 during the long outage for the proton power upgrade (PPU) at SNS. The STS development beamline would then become available for use around the ends of 2024.

6. INSTRUMENT SPECIFIC R&D

Several instruments at the STS will utilize new concepts and components that require research and development to ensure that they work as expected and can function reliably as part of an operating user facility. The WAVES rotor a key part of the BWAVES instrument is one such example.

6.1 INITIAL WAVES ROTOR TESTING FOR THE BWAVES INSTRUMENT

BWAVES is an acronym for Broadband Wide-Angle VElocity Selector spectrometer, indicating that a novel WAVES (Wide-Angle VElocity Selector) device will be used to select the velocity/wavelength of the detected neutrons after the sample scatters them (Mamontov *et al.*, 2022). An existing prototype WAVES rotor (Prototype 1) optimized for use with 3.36 Å neutrons was developed as part of a previous LDRD project. This rotor has undergone rotational testing, where it performed as expected. However, testing with neutrons has not occurred due to complications in accessing a suitable beamline at SNS. A protective box will be constructed to enable testing with neutrons that encases the WAVES rotor protecting the host beamline from damage in case of a malfunction with the WAVES rotor. Initial testing of the first WAVES rotor is now planned at the VULCAN beamline at SNS. Testing the existing WAVES rotor will occur in parallel with the WAVES rotor R&D effort for the BWAVES instrument. Initial testing will be aimed at verifying several theoretical predictions regarding the performance of a WAVES rotor, which are central to the design of a new WAVES rotor for the BWAVES and for the design of the BWAVES instrument itself. In particular, the theoretical dependence of the energy resolution of the existing WAVES rotor on the following operation parameters needs to be tested: (a) the rotor rotation frequency, (b) the sample size, (c) the in-plane scattering angle component, and (d) the out-of-plane-scattering angle component. The testing of the Prototype 1 WAVES rotor is planned to take place in FY23.

6.2 WAVES ROTOR R&D FOR THE BWAVES INSTRUMENT

Novel approaches necessary for implementing a WAVES device at the BWAVES spectrometer will result in a spectrometer with the design and characteristics much different from those displayed by the neutron spectrometers in existence today. In essence, a high energy-resolution broadband spectrometer will have an open-access sample geometry more resembling that of neutron reflectometers than spectrometers.

As the device for selecting the final neutron velocity, v_f (wavelength, λ_f), the WAVES rotor is the most critical component of the BWAVES spectrometer (Figure 12). However, such a device has not been tested with neutrons to date. Thus, the main driver for this R&D project is to manufacture and test with cold neutrons a WAVES rotor similar to the one that will be deployed on the BWAVES instrument.

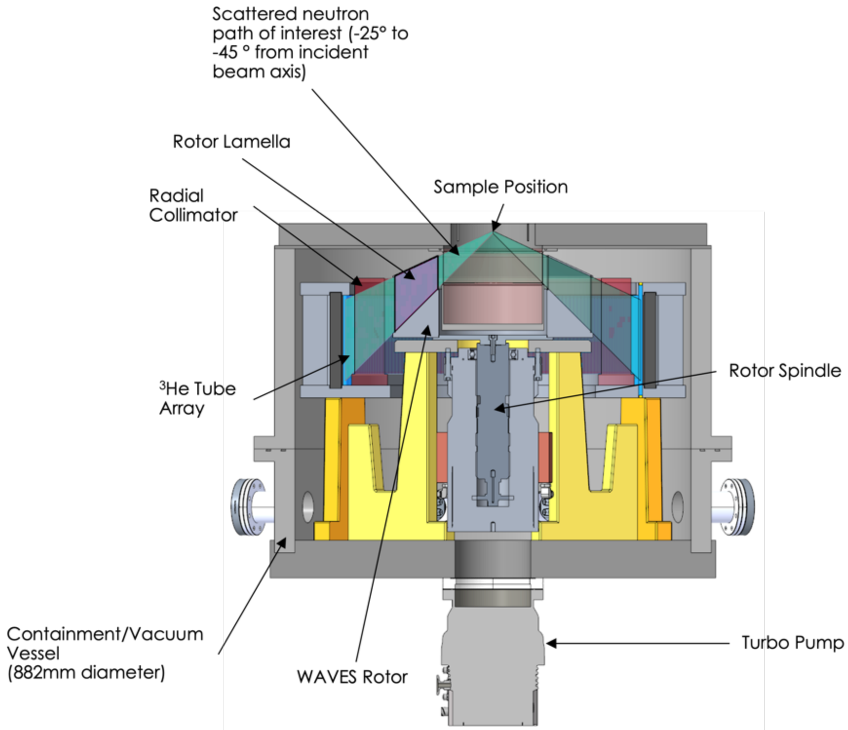

Figure 16: Current engineering model of the BWAVES Detector/Rotor vacuum vessel

This rotor will be optimized to transmit neutrons with a final wavelength of 14.5 Å. The steps to be taken in the framework of this R&D effort will be as follows.

1. A feasibility design study by the vendor of a Prototype 2 WAVES rotor. Such a design study is necessitated by substantial differences between the existing Prototype 1 WAVES rotor and the future Prototype 2 WAVES rotor. The main difference is that the Prototype 2 WAVES rotor will be optimized for use with the current design of the BWAVES instrument, requiring $\lambda_f = 14.5$ Å (hence, ca. five times longer blades compared to the Prototype 1 WAVEs rotor) and a range of out-of-plane scattering angles between 25 and 45 degrees. Therefore, both much longer and taller neutron absorption blades are to be used for the Prototype 2 WAVES rotor, which thus will experience a much greater deformation force. This will likely make the implementation of wedged-shape aluminum spacers between the rotor blades unavoidable. Since such spacers have not been used for the Prototype 1 WAVEs rotor, an entirely new finite element-based analysis will need to be undertaken by the vendor to find a way to keep the deformation of the blades within the acceptable limits while simultaneously minimizing attenuation of the scattered neutrons through the spacers on their way to the detectors. This R&D task is to start in FY22 and finish in FY23.
2. Based on the findings and recommendations of the feasibility design study, the design is to be optimized and procurement issued for the Prototype 2 WAVES rotor before the end of FY23. We expect this R&D task to be guided by the feasibility design study and the Prototype 1 WAVES rotor testing.
3. The design and procurement of a test vessel for the Prototype 2 WAVES rotor (FY23-24, while the rotor is being manufactured)

4. Testing of the Prototype 2 WAVES rotor at the STS development beamline (as it cannot be carried out at VULCAN that lacks neutron flux at long wavelengths such as λ_f = 14.5 Å). The timeframe for completing this R&D task is FY25, contingent upon the availability of the STS development beamline.
5. Based on the findings from testing the Prototype 2 WAVES rotor, further modifications of the rotor design are to be made and procurement issued for Prototype 3 WAVES rotor (FY 25-26) which is intended to be fully representative of the final device procured during the project execution phase.
6. Testing the Prototype 3 WAVES rotor at the STS development beamline (FY 26). If the test results demonstrate satisfactory performance, this R&D effort will be concluded. The specification for Production Article 1 WAVES rotor for the BWAVES instrument can be prepared based on Prototype 3 WAVES rotor.

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