

ANL/IPNS/CP-96861
CONF-980921--
RECEIVED
JUL 30 1999
OSTI

NEUTRON SCATTERING INSTRUMENTS FOR THE
SPALLATION NEUTRON SOURCE

R. K. Crawford
Argonne National Laboratory and the
Spallation Neutron Source Project
Argonne, IL 60439 USA
(630) 252-7769

K. W. Herwig
Oak Ridge National Laboratory and the
Spallation Neutron Source Project
Argonne, IL 60439 USA
(630) 252-5371

ABSTRACT

The Spallation Neutron Source (SNS) is an accelerator-based short-pulse neutron scattering facility designed to meet the needs of the neutron scattering community in the United States well into the next century. SNS is a U.S. Department of Energy (DOE) construction project that is planned to be completed at Oak Ridge National Laboratory late in 2005. SNS is being designed and will be constructed by a 5-laboratory collaboration including Argonne National Laboratory, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory and Oak Ridge National Laboratory. The functional requirements for the SNS have been set by the scientific community and DOE.

In operation, the SNS accelerator system will produce very short ($<1 \mu\text{s}$) intense pulses of protons at a 60 Hz rate. These proton pulses bombard a mercury target, producing large quantities of fast neutrons by the spallation process. Two ambient temperature water moderators and two cryogenic liquid hydrogen moderators slow the neutrons from the target to produce beams of thermal and cold neutrons optimized for neutron scattering experiments.

SNS will initially operate at 1 MW with one target station operating at 60 Hz and having 18 beam ports for neutron scattering experiments. The first 10 neutron scattering instruments are provided as part of the SNS construction project, and will be selected to span the types of science anticipated to be most important for this facility on the basis of input from the user community. These 10 instruments are expected to be installed and ready for commissioning at the time the source turns on (late 2005). It is expected that additional instruments will be installed soon after that.

This paper describes the process of selection and design of these first 10 instruments. The extensive R&D program to support the design and construction of these instruments and to help pave the way for future instruments will also be discussed. A set of 10 "reference instruments" has been developed to help establish the layout of the experiment hall and the interface between the instruments and the target station. This layout and some of the associated interface issues will be described. Examples of the design and performance of some of these reference instruments will also be discussed as an indication of the types of instrumentation involved and the new scientific capabilities that should be available when the SNS becomes operational.

Work supported in part by the U. S. Department of Energy, BES, contract No. W-31-109-ENG-38.

The submitted manuscript has been authored by a contractor of the U. S. Government under contract No. W-31-109-ENG-38. Accordingly, the U. S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U. S. Government purposes.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

**Portions of this document may be illegible
electronic image products. Images are
produced from the best available original
document.**

I. OVERVIEW OF THE SNS FACILITY

The Spallation Neutron Source (SNS) is an accelerator-based facility designed to meet the needs of the neutron scattering community in the United States well into the next century. SNS is a U.S. Department of Energy (DOE) project that is being designed and will be constructed at Oak Ridge National Laboratory by a collaboration including Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Lawrence Berkeley National Laboratory (LBNL), Los Alamos National Laboratory (LANL) and Oak Ridge National Laboratory (ORNL). The functional requirements for the SNS have been set by the scientific community in conjunction with DOE.

In operation, a front-end system and a linac produce and accelerate large currents of H^+ ions to 1 GeV. A stripping process is used to inject these ions into a proton accumulator ring, where they are collected and then extracted as very short ($<1 \mu s$) intense pulses of protons. These proton pulses bombard a mercury target, producing large quantities of fast neutrons by the spallation process. Two ambient temperature water moderators and two cryogenic supercritical hydrogen moderators slow the neutrons from the target to produce beams of thermal and

cold neutrons optimized for neutron scattering experiments. This facility is fully described in a Conceptual Design Report.¹ Figure 1 shows the proposed facility configuration. LBNL is responsible for the front end, LANL for the linac, BNL for the accumulator ring, ORNL for the target station, and ANL for the neutron scattering instruments.

SNS will initially operate at 1 MW and 60 Hz with one target station having 18 beam ports. The construction project provides funding to design and construct ten instruments for neutron scattering experiments. Upgrade paths have been identified for providing additional instruments, a second target station operating at 10-20 Hz, and substantial increases in power. The eventual configuration with two target stations will provide at least 36 fully-instrumented neutron beams, and ultimate accelerator power of at least 4 MW. This upgrade process is designed to allow SNS to grow as the needs of the scientific community expand.

Construction of the SNS facility will require 7 years, starting in October, 1998. Total project cost is \$1,333 M, of which \$59 M is for construction of the ten neutron scattering instruments and \$24 M is for instrument R&D.

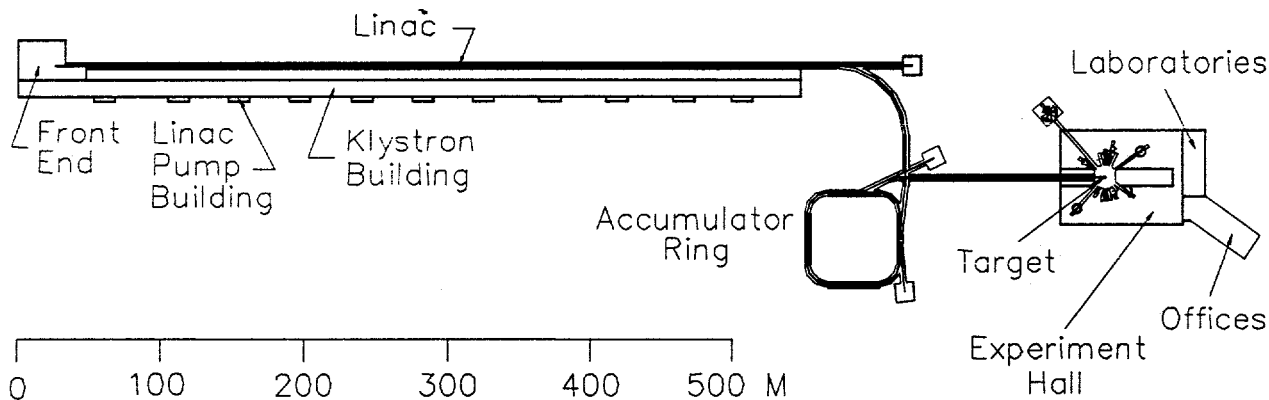


Figure 1. Proposed layout of the SNS facility.

II. SELECTION, DESIGN, CONSTRUCTION, AND INSTALLATION OF INSTRUMENTS

As noted above, the SNS construction project contains funding for design and construction of the first ten neutron scattering instruments. These will be selected on the basis of input from the user community, and will span the types of science anticipated to be most important

for this facility. These ten instruments will be installed and ready for commissioning at the time the source turns on late in 2005. It is expected that additional instruments will be installed soon after that.

The broad user community will be involved in the selection, design, construction, and operation of the neutron scattering instruments. This involvement has

already begun. A workshop held in October 1996 provided user recommendations for more than 30 neutron scattering instruments to support the different types of science. A second user workshop is scheduled for Fall, 1998. This workshop will lead to the formation of Instrument Advisory Teams made up of scientists with interests in specific types of instruments. These teams will formulate concepts for the different instruments. An Instrument Oversight Committee of external scientists will then advise SNS management about which of these concepts should be selected for design and construction.

Argonne National Laboratory, working with scientists from Oak Ridge National Laboratory, is responsible for the design, construction, and installation of the first ten neutron scattering instruments. The Instrument Advisory Teams will play a major role in this process as well. Each instrument will have an associated scientist responsible for directing the design and construction effort. These instrument scientists are currently being hired by ORNL. They will be stationed at ANL and work with experienced ANL scientists during the design and construction phases, and will then move to ORNL to supervise installation of the instruments. When the facility is operational, these scientists will be the "instrument scientists" responsible for the operation of these ten instruments for the users. This process will ensure that the facility will have a core of trained scientists to enhance its effectiveness as a user facility.

III. RESEARCH AND DEVELOPMENT

The \$24 M earmarked for instrument-related R&D activities is intended not only to support the design and construction of the first ten instruments, but also to enhance the infrastructure for the development of future instruments. This R&D effort is divided into the nine separate categories described briefly below.

A. Instrument Specification

This task concerns the development and refinement of concepts for a variety of neutron scattering instruments, and is intended to provide the basis for selecting the ten instruments to be built as part of the construction project. Instrument Advisory Teams will provide extensive user input into this process. Instruments in use at existing pulsed neutron facilities, particularly ISIS, will be studied and used as starting points for some of the concepts. Other documentation such as the IPNS upgrade study and various European Spallation Source studies may lead to additional concepts. Coordination will also take place with the LANSCE instrument upgrade. Prototyping of some of these instrument concepts will be

carried out at IPNS and LANSCE, and possibly at other facilities.

B. Design Tool Development

This task involves the development of software tools for design of neutron scattering instruments. Primary emphasis will be placed on the development of Monte Carlo codes for simulating the performance of the different kinds of instruments. These codes will be developed as a set of modules for individual neutron optical components, so that these modules can then be linked together to simulate an entire instrument. In this way a small number of optical component code modules can provide the basis for a large variety of instruments simply by changing the linking of the modules. SNS will work with the international community to set standards for such modules so that modules developed at various other facilities can be readily used. In this way not all of the necessary code need be supplied by SNS. A workshop has already been held to initiate this process.² This Monte Carlo software suite will be used in the instrument evaluation process and in the optimization of the instruments. Development of this software will continue to the point where the software is useful in diagnosing problems during the instrument commissioning phase, and in designing experiments and interpreting data once the instruments are operational.

C. Concept Evaluation and Instrument Selection

The Monte Carlo simulation codes and other design tools will be used to model the most promising of the instrument concepts. Full simulations based on these models will be used to evaluate the relative performance of the different concepts. This information will serve as input for the process of selecting the ten instruments to be constructed, which will involve the Instrument Advisory Teams, the Instrument Oversight Committee, and SNS management.

D. Data Acquisition System Development

The heart of all the time-of-flight neutron scattering instruments at SNS will be the system that collects the pulses from the detectors and histograms these pulses in a manner that is meaningful to the instrument user. Each of these instruments will collect data from 10^2 to 10^5 detector pixels, each of which is further resolved into 10^2 to 10^4 time-of-flight channels. In some cases other parameters such as the chopper phase or state of a time-varying field on the sample will also be important. Data rates will be very high on many of the SNS neutron scattering instruments, and all of these instruments will collect and

histogram many channels of this multi-parameter data. A new generation of data acquisition system must be developed to meet these requirements. Development of this system will involve construction and testing of prototype systems using realistic conditions on existing pulsed neutron source instruments at IPNS and LANSCE.

E. Neutron Detector Development

Instruments at pulsed sources can utilize many detectors to simultaneously acquire data at different angles. Standard ^3He detectors are generally satisfactory, but are very expensive. In some cases desired data accumulation rates and the need for very high spatial resolution are not possible with existing technology. Scintillation detectors look promising, but still have some problems. Recent work indicates that solid state detectors may also be useful for some applications. Development work will be done to improve the performance of scintillation detectors, to investigate the applicability of solid state detectors, and to produce position sensitive detectors with a high spatial sensitivity and capable of a high count rate. Activities likely to reduce the cost of neutron detectors will also be supported. A SNS Detector Advisory Committee composed of experts external to the project has been formed to provide advice concerning choices of technology and vendors for detector R&D.

F. Neutron Chopper Development

Almost all of the neutron scattering instruments will require neutron choppers of various types. T_0 choppers are used to remove the burst of fast neutrons associated with the prompt pulse, bandwidth choppers restrict the wavelength range of neutrons allowed to reach the detectors, and E_0 choppers are used to select the incident neutron energy in chopper spectrometers. T_0 choppers that can fit within the space in the SNS chopper caves must be developed. T_0 and bandwidth choppers must be developed that can minimize the background in the instruments even when some of the pulses are being eliminated. High-speed E_0 choppers must be developed to provide the best timing resolution for chopper spectrometers. Suitable electronic systems for controlling these choppers must also be developed.

G. Sample Environment Development

The SNS will make very rapid data collection possible for some experiments. With present equipment it may take longer to change the sample environment (for instance the temperature) than to accumulate the data. In order not to waste neutrons, equipment will have to be developed to make rapid and accurate changes in the

sample environment. Additional capabilities for affecting the sample environment will also be developed to enhance the scientific effectiveness of the neutron scattering instruments. These capabilities include specialized cryostats, furnaces, magnets, high pressure cells, etc.

H. Neutron Optical Component Development

Advances in optics can greatly increase the counting rates for some experiments. Long neutron guides will be required for several of the instruments and development in supermirror technology can reduce their cost and improve their performance. Focusing optics for neutrons, including elliptical mirrors with supermirror or stable isotope coatings and neutron lenses of various types will also be developed to enhance the neutron flux on the samples where practical. Polarized neutrons provide many opportunities to extract additional information from the neutron scattering samples. Polarizers will have to be developed that will polarize a wide energy spectrum of neutrons. A program will be undertaken to improve present day polarizers. Since good polarizers are needed at all pulsed sources joint programs with other Laboratories will be established. Other equipment for manipulating the polarized neutrons will be developed as needed. A SNS Optical Component Advisory Committee composed of experts external to the project will provide advice concerning choices of technology and vendors for optical component R&D.

I. Data Analysis and Visualization Software

The SNS instrumentation will acquire data simultaneously at many different momentum and/or energy transfers. In order to proceed optimally with an experiment, data will have to be examined as the experiment is in progress. As noted above, some of the spectrometers will acquire more than 10^6 data points each run. Furthermore, the run times could be as short as a few minutes for some of the spectrometers. Data from the runs have to be visualized in an effective way to use the beam time properly. In some cases the data will have to be converted to the parameters of interest such as a bond length or an energy transfer along a given crystal direction. Computer programs will be developed to enable rapid visualization of raw or partially reduced data. Programs will also be required for full reduction and analysis of the data after it is collected. In some cases totally new approaches will have to be developed to make efficient use of all the information in the data sets.

IV. THE REFERENCE SET OF INSTRUMENTS

A. Overview

The recommendations of the first User Workshop have been distilled to define a reference set of ten instruments to be used for planning purposes, and reference design concepts have been prepared for this set. Table 1 lists this reference set. Each instrument selected is one of the highest priority instruments specified at the workshop and is capable of effective operation at the 60-Hz target station. Instruments in the reference set span a very wide and representative range of science and a representative range of instrument types and costs. More detailed information about these ten reference instruments can be found in the SNS Conceptual Design Report.¹

A layout of this reference set of instruments on the neutron beams was developed to provide a realistic optimization of the configuration of the experiment hall and to define in detail a suitable interface between realistic instruments and the target station, including shielded locations for choppers. Figure 2 shows the optimized layout of this reference set of instruments in the experiment hall based on these reference instrument conceptual designs. In this layout each instrument views its appropriate moderator and the high-resolution powder diffractometers view their respective moderators at normal incidence in order to provide the best time-of-

flight resolution. Side access to instruments is preserved wherever possible, with as many as practical of the instruments lying under crane coverage within the experiment hall. These reference instruments have also been subjected to a careful cost and schedule analysis to make sure the planned budget and schedule for the instruments is realistic.

B. Performance

Table 1 also gives an indication of typical measurement times to be expected if the reference instruments were operated at the 1 MW SNS. These measurement times are estimated by scaling from existing instruments at ISIS and IPNS, taking into account the differences in source flux, detector solid angle, guide performance, etc. These times are intended only as a rough indication of what would be possible at SNS. In reality, measuring times will be different for the suite of instruments actually built and installed at SNS, and will depend strongly on the specific samples being studied and the types of information required. An instrument specifically optimized to provide the highest data rates for real-time measurements could achieve much shorter measuring times than these, at some expense in resolution.

Table 1. Reference Set of Instruments

Label	Description	Resolution (fwhm)	Incident Path (m)	Typical Measuring Time (min)
POW3	General purpose powder diffractometer	$\Delta d/d = 0.0013$	30	30
POW6	High-resolution engineering powder diffractometer	$\Delta d/d = 0.0007$	60	150
POW7	Glasses/liquids diffractometer	$\Delta Q/Q = 0.007-0.1$	9	10
SCD1	General purpose single crystal diffractometer	$\Delta d/d = 0.005$	12	20
SANS2	General/lower-Q high resolution SANS	$Q_{\min} = 0.001 \text{ \AA}$	17	30*
REF1	Horizontal-surface reflectometer	$\Delta q/q = 0.02-0.1$	12	20
INEL1	Microvolt spectrometer	$\Delta E = 5 \text{ } \mu\text{eV}$	31	20
INEL2	100-microvolt spectrometer	$\Delta E = 70 \text{ } \mu\text{eV}$	12	5
INEL4	Wide-angle chopper spectrometer	$\Delta E/E = 0.01$	18	120
INEL5	Large-solid-angle single-crystal spectrometer	$\Delta E/E = 0.01$	15	120

* For a strong scatterer

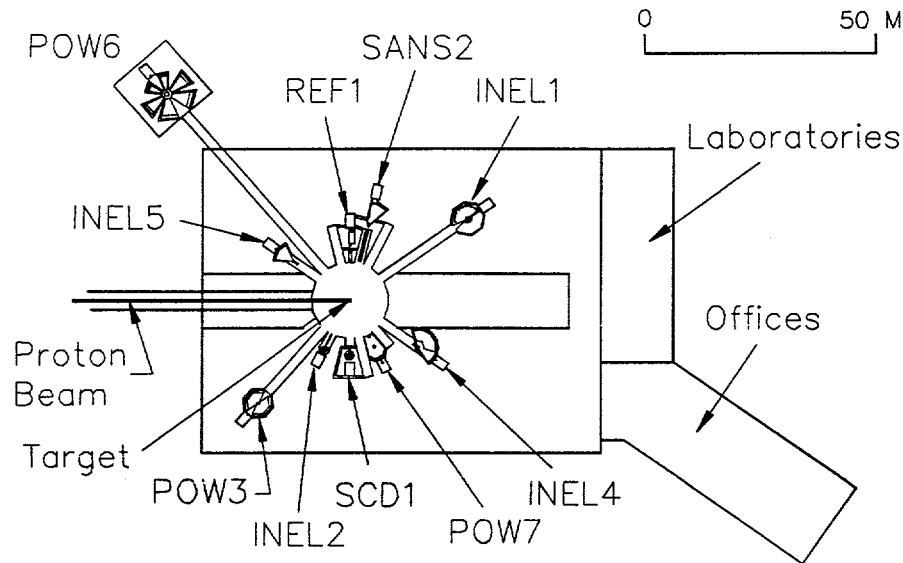


Figure 2. Layout of the reference set of instruments in the SNS experiment hall.

C. Design Issues

The layout of the reference set of neutron scattering instruments in the experiment hall and the interfacing of these instruments with the target station design has identified a number of design and component development issues. Where appropriate, these have been incorporated in the R&D program described above. Other issues are being considered in the design of the experiment hall and the target station. A few of the latter are discussed here.

The extensive need for choppers has been integrated into the design of the target station shielding, which incorporates shielded cavities in each beam line to allow insertion of T_0 and bandwidth choppers as needed. This approach should provide better shielded areas for the choppers and tighter beamline shielding.

There will be a continuing interplay between the instrument designers and the designers of the neutron moderators in the target station. Moderator properties must be matched to the needs of the instruments, and the reference instrument set has played a vital role in identifying some of these needs at an early stage.

Neutron guides will be used on many of the instruments. In some cases a fully-optimized guide system will require that the guide extend relatively close

to the moderator (<5 m). In this region the guide must extend through the shutter (2.5 m to 4.5 m from the moderator) and perhaps extend into the sealed inner tank in the target station (<2.5 m) where cooling and radiation damage will be important. The target station is being designed to accommodate these needs to the extent practical. Design, installation, and maintenance of these portions of the guides will be a challenge.

V. STATUS AND SCHEDULE

The President's budget for FY99 includes funding for a line item construction start for the SNS project. This budget is now proceeding through Congress, and if this item is approved, the construction project will start in October, 1998. The Instrument Advisory Teams and the Instrument Oversight Committee will be formed in late 1998. Plans then call for all ten of the instruments funded by the project to be selected by October, 2000, with some instruments being selected prior to that time. Instrument construction and installation at the SNS facility in Oak Ridge will be complete by October, 2005, which marks the end of the construction project and the beginning of facility operation and instrument commissioning.

VI. SUMMARY

In summary, the SNS short-pulse spallation source will provide a significant increase in the neutron

scattering capabilities in the U.S. This facility is planned to be available late in 2005, and the user community is encouraged to begin thinking now about the types of instrumentation desired for this facility. A substantial R&D program is planned to complement the instrument construction effort and to enhance the infrastructure for the development of future instruments. This R&D activity should also benefit other neutron scattering facilities worldwide.

REFERENCES

1. The SNS Collaboration, *Spallation Neutron Source Conceptual Design Report*, Oak Ridge National Laboratory report SNS/CDR-2, Oak Ridge National Laboratory, Oak Ridge, Tennessee (1997).
2. R. K. Crawford, *Report on the Workshop on Monte Carlo Simulation of Neutron Scattering Instruments*, Argonne National Laboratory, November 13-14, 1997. SNS Technical Note ANL/SNS/97-2, Argonne national laboratory, Argonne, Illinois (1997).