

## IPNS NEUTRON SCATTERING INSTRUMENTATION

## A. EXISTING AND PLANNED

## B. POSSIBILITIES FOR IPNS UPGRADE, A 1-MW SPALLATION SOURCE

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The Intense Pulsed Neutron Source (IPNS) is a pulsed spallation neutron source located at Argonne National Laboratory near Chicago, Illinois in the U.S. This facility is the outgrowth of a long line of pioneering work on pulsed spallation neutron sources begun at Argonne in the early 1970s. IPNS uses protons accelerated in the Rapid Cycling Synchrotron to produce neutrons via the spallation process (effectively a nuclear "evaporation" in which 10-50 neutrons are released per incident proton) in a heavy-element target. These neutrons are then moderated to produce spectra peaked at thermal or subthermal energies, and directed into beams which serve a variety of instruments. Figure 1 shows a layout of the accelerator and target system.

From the initial operation in 1981, IPNS has been operated as a National User Facility; IPNS is currently running the 23rd round of user proposals. Table I lists the number of experiments and users at IPNS as a function of fiscal year. For most instruments, 75% of the beam time is allocated by a Program Advisory Committee (PAC) on the basis of proposals submitted by the users, and 25% is reserved for the Instrument Scientists. The PAC, which meets twice a year, also allocates 25% of the beam time on the instruments built by Participating Research Teams (PRTs), with the remainder being allocated by the PRT to its members. Most instruments have been oversubscribed by factors of 2-3 since their commissioning, and no instruments are undersubscribed. The PAC always has a majority of non-Argonne members, with its membership chosen to span the diversity of types of science typically proposed. For experiments accepted by the PAC done in collaboration with the Instrument Scientist, or allocated within the framework of a PRT, the neutron beam time and the use of the relevant IPNS instrument, analysis codes, and computing facility are provided free of charge for publishable research. Some support is also available from the University of Chicago Board of Governors for Argonne to cover travel and lodging for university users. Beam time for proprietary work or for publishable work which is not accepted by the PAC can be purchased under a rate structure established by the Department of Energy.

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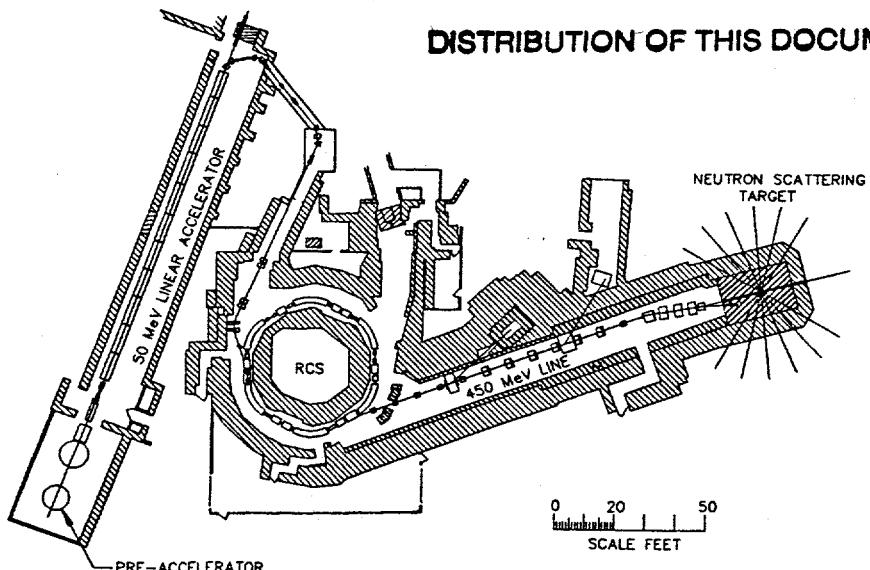


Figure 1. Layout of the IPNS accelerator system and the neutron scattering target station.

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Table I—IPNS USER PROGRAM

FY82 FY83 FY84 FY85 FY86 FY87 FY88 FY89 FY90 FY91 FY92 FY93 FY94

NO. OF EXPERIMENTS PERFORMED	94	110	210	180	212	223	257	323	330	273	210	248	281
VISITORS TO IPNS FOR AT LEAST ONE EXPERIMENT:													
ARGONNE	37	41	49	44	52	55	57	60	61	60	53	48	49
OTHER GOV. LABS	8	9	8	7	11	15	18	16	19	15	14	18	13
UNIVERSITIES	27	33	45	51	79	78	89	94	120	92	62	64	63
INDUSTRY	5	5	9	7	13	24	20	24	36	18	20	16	15
FOREIGN	12	18	39	35	27	24	17	26	18	27	14	25	32
	89	106	150	143	182	196	201	220	254	212	163	171	172
NO. OF USER INSTRU.	4	5	6	6	6	6	6	7	7	7	7	6	6
NO. OF "PRT" INSTRU.	1	1	1	2	3	3	4	4	5	5	5	6	6

Essential to the effective operation of IPNS as a facility for outside users has been the extremely high reliability of the accelerator system. IPNS has always been extremely proud of its operating reliability (defined as the percentage of scheduled operating time during which the accelerator, target, and moderators are all functioning to deliver useful beams to the instruments). From the beginning, the operating reliability of IPNS has been consistently around 90% or higher; and, in recent years, this has increased to values around 95% on an annual basis. This high reliability has made it possible for users to schedule their visits and count on being able (in nearly all cases) to collect their data during their scheduled visit. In those few cases where problems are encountered in neutron source operation, in operation of the specific instrument, or in the user's own equipment, the dedicated operation of the accelerator system has usually permitted the flexibility to accommodate to the scheduling changes necessary to complete the experiment (for example, by extending the run).

Despite its dedication to operation for a user program, IPNS has also continued the tradition of innovative developments in the technology of pulsed neutron sources and instrumentation begun with the IPNS prototypes almost two decades ago. Most neutron scattering instruments in operation at pulsed sources today had their first version developed and operated at IPNS. A number of different cryogenic polyethylene, methane (both liquid and solid), and hydrogen (liquid) moderators have been installed, operated, and characterized.

Contrary to a widely held belief, pulsed neutron sources are actually excellent for applications requiring the use of cold neutrons. Moderator heating is a much less severe problem at pulsed sources, so unlike the situation at most reactors, cold moderators at pulsed sources can be located in the positions of maximum flux. As a consequence, large cold-neutron fluxes can be produced, and many of the IPNS instruments described below use cold neutrons extensively. The reflectometers POSY and POSY-II and the small-angle diffractometers SAD and SAND all routinely and effectively use neutrons at wavelengths out to 14 Å. The inelastic scattering instruments QENS and HRMECS can both achieve energy resolution of about  $70\text{ }\mu\text{eV}$  when using 5 Å neutrons, and virtually all of the QENS measurements are based around this wavelength. Although HRMECS is effective over an extremely broad range of energies, cold neutron measurements occupy a constantly-increasing fraction of the time on HRMECS as well.

In October, 1988, the original depleted uranium neutron scattering target was replaced with a 77% enriched uranium (Booster) target. This first-ever use of a Booster target at a spallation neutron source was the culmination of massive efforts in design, in safety analysis, and in fabrication technology, and resulted in a nearly three-fold increase in the available neutron flux at the neutron scattering instruments. The impact of the backgrounds due to the

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increased number of delayed neutrons associated with the Booster target has been successfully controlled by software measures and by the use of delayed-neutron-removing choppers. A leak in 1991 required removal of the target and the return to depleted uranium, but a new Booster target has been designed and the goal is to install it within the next year.

## A. INSTRUMENTS EXISTING AND PLANNED FOR IPNS

Figure 2 shows the instruments now operating or under development at IPNS. Table II summarizes some specifications for these instruments, which are discussed in greater detail below.

The two powder diffractometers (SEPD - Special Environment Powder Diffractometer, GPPD - General Purpose Powder Diffractometer<sup>1</sup>) coupled with the variety of available ancillary equipment and the on-line capability of the Rietveld profile refinement method have proven to be excellent instruments for structure refinements, and have always been heavily oversubscribed. Samples studied have included ceramics, hydrides, metal alloys, metallic glasses, oxides, and organic materials, and measurements have been made at a wide variety of temperatures (0.2 - 1700 K) and pressures (up to 25 kbar). As one might expect, over the past several years a significant fraction of the time on these instruments has been allocated to structural and defect studies of the high- $T_c$  superconductors. Considerable work has also gone into the determination of residual strains in composite materials. In recent years, an increasing variety of automated ancillary equipment (furnaces, sample changers, etc.) has greatly increased the throughput of these instruments.

The High Intensity Powder Diffractometer (HIPD) was built to study surface diffraction from molecules adsorbed on large-surface-area substrates. The total amount of sample present in the adsorbed layers in these systems is small; and, these types of studies do not require high resolution, so the instrument has been designed to sacrifice resolution to provide intensities as high as practical. A low-angle detector bank results in resolution ranging from 1.8% to 3.5% and a second detector bank at 90° has resolution of 0.95%. This instrument has been very productive for the measurement of adsorbed species, and since the 90° bank has been added it has also been useful for Rietveld refinements on certain classes of crystalline materials. The low-angle bank has also been particularly well suited to the study of magnetic structures. Most of the standard IPNS furnaces, refrigerators, and cryostats are available for use on this instrument.

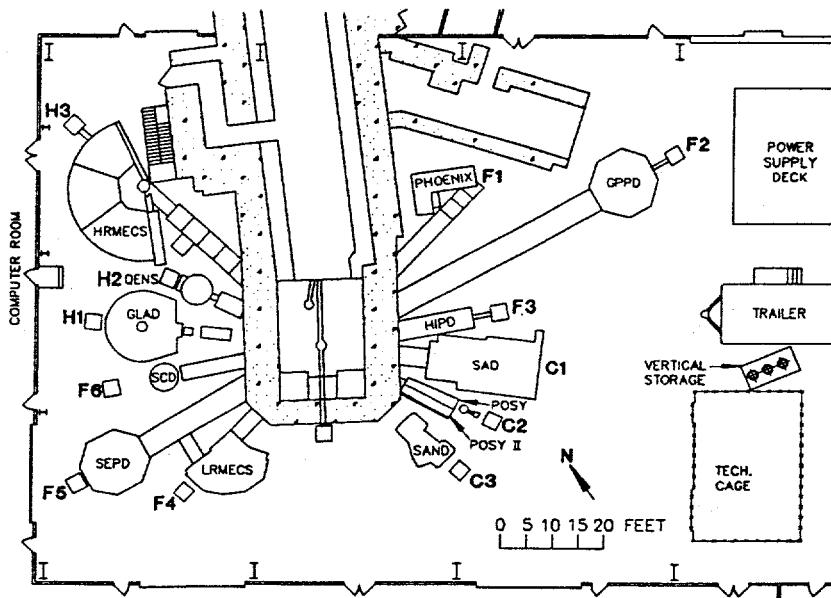


Figure 2. The IPNS Experimental Hall showing the layout of the neutron scattering instruments

Table II—IPNS NEUTRON SCATTERING INSTRUMENTS

Instrument (Instrument Scientist)	Range Wave-vector* ( $\text{\AA}^{-1}$ )	Range Energy (eV)	Resolution Wave-vector ( $\text{\AA}^{-1}$ )	Resolution Energy (eV)
<b>Special Environment Powder Diffractometer</b> (J. D. Jorgensen/R. Hitterman)	0.5-50	**	0.35%	**
<b>General Purpose Powder Diffractometer</b> (J. Richardson//R. Hitterman)	0.5-100	**	0.25%	**
<b>Single Crystal Diffractometer</b> (A. J. Schultz/R. Goyette)	2-20	**	2%	**
<b>Low-Resolution Medium-Energy Chopper Spectrometer</b> (R. Osborn/L. Donley)	0.1-30	0-0.6	$0.02 k_0$	$0.05 E_0$
<b>High-Resolution Medium-Energy Chopper Spectrometer</b> (C.-K. Loong/J. Hammonds)	0.3-9	0-0.4	$0.01 k_0$	$0.02 E_0$
<b>Small Angle Diffractometer</b> (P. Thiagarajan/D. Wozniak)	0.006-0.35	**	0.004	**
<b>Low-Temperature Chopper Spectrometer</b> (P. E. Sokol--Penn State University, 814/863-0528)	0.3-30	0.1-0.8	$0.01 k_0$	$0.02 E_0$
<b>Polarized Neutron Reflectometer (POSY)</b> (G. P. Felcher/R. Goyette)	0.0-0.07	**	0.0003	**
<b>Neutron Reflectometer (POSY II)</b> (A. Wong/R. Goyette)	0.0-0.25	**	0.001	**
<b>Quasi-Elastic Neutron Spectrometer</b> (F. Trouw)	0.42-2.59	0 - 0.1	-0.2	$70 \mu\text{eV}^{\$}$ $0.01 \Delta E$
<b>Glass, Liquid and Amorphous Materials Diffractometer¶</b> (D. Price/K. Volin)	0.05-25 0.1-45	** **	$\sim 0.5\% \cot \theta$ $\sim 1.0\% \cot \theta$	** **
<b>High Intensity Powder Diffractometer</b> (F. Trouw)	0.5-25 1.8-50	** **	1.8-3.5% 0.9%	** **

\* Wave-vector,  $k = 4\pi \sin \theta / \lambda$

\*\* No energy analysis

¶ Two sample positions

§ Elastic and inelastic resolution

NOT CURRENTLY IN THE USER PROGRAM

Small Angle Neutron Diffractometer (SAND, under development)

Until recently, neutron diffraction measurements of the structure of disordered materials at pulsed sources were carried out on diffractometers such as SEPD and GPPD, which are quite useful for structural studies of glasses and liquids due to the abundance of epithermal neutrons and hence of high-Q data at pulsed neutron sources. While much work of high quality was carried out, these instruments fall far short of meeting the requirements for state-of-the-art structure measurements on disordered systems. Because of this, a few years ago a group of Argonne and university scientists, organized as a PRT led by the University of Houston, decided to build a new instrument optimized for structural measurements in glasses and liquids at IPNS. This new instrument, the Glass, Liquids, and Amorphous Materials Diffractometer (GLAD), has now been commissioned and the first scientific measurements have been carried out. Details of the performance of this instrument, including background, calibration, resolution, data rate, data quality, and data reduction and analysis have been discussed elsewhere.<sup>2</sup>

Analysis of neutron scattering from materials containing light atoms is plagued by the importance of inelasticity corrections. Therefore, GLAD was designed to collect data over as broad a Q-range as possible using the highest energy neutrons collected over the smallest range of scattering angles, and to perform these experiments in the extremely limited amount of time typically allotted to experimenters. GLAD routinely collects data at neutron wavelengths between 0.05 Å and 5 Å, and can obtain reliable data for scattering angles between 4° and 95° (higher for the downstream sample position). For difficult samples, the data analysis can be restricted to a subset of the angles and wavelengths to improve the quality of the data and minimize corrections. For example, an excellent-quality structure factor of D<sub>2</sub>O out to 30 Å<sup>-1</sup> was obtained using detector segments from 8-30° over a wavelength range of 0.1 - 1.0 Å. When a broader range of scattering angles and/or a larger wavelength range can be employed, the statistics at all points are improved significantly, and the structure factor data can be extended to far higher Q (analyses are routinely performed using data through Q = 40 Å<sup>-1</sup>, and occasionally to Q = 50 Å<sup>-1</sup>).

GLAD is by far the most technically sophisticated instrument at IPNS, with two sample positions and 235 linear position-sensitive detectors (LPSDs) distributed about these sample positions. The use of LPSDs permits GLAD to handle high data rates and to cover low scattering angles. Crossed converging soller collimators focused on the forward detector bank collimate the thermal and epithermal neutrons used by GLAD. With this collimation scheme, the sample size does not contribute significantly to the resolution, so large samples can be used. Considerable attention has been given to sources of background in GLAD; and, over the wavelength range for which GLAD is optimized, its background is currently the lowest among diffractometers at IPNS. The data files are large and a typical experiment results in several such files generated in a short period of time, so efficient programs have been developed for analyzing the data and compressing it to more manageable sizes.

The Single Crystal Diffractometer (SCD)<sup>3</sup> uses the time-of-flight Laue technique for diffraction measurements on single crystals. Data are collected with a two-dimensional (30 x 30 cm) position-sensitive scintillation detector (neutron Anger camera) developed and built at Argonne and having ~3 mm resolution. The SCD sample is oriented by a four-circle goniostat under computer control. Ancillary environmental equipment permits a range of temperatures (4 - 1000 K) and pressures (0 - 5 kbar). The SCD is routinely used for structure determinations with single-crystal samples, as well as for a variety of problems relying on its ability to quickly investigate large regions of reciprocal space. The area detector and the range of wavelengths from the pulsed source provide a three-dimensional sampling of reciprocal space with a single orientation of the sample, and this is extremely useful in studies of diffuse scattering, in texture determination, and in characterizing nuclear and magnetic phase transitions and the measurement of incommensurate satellite reflections.

The Small Angle Diffractometer (SAD)<sup>4,5</sup> also includes a two-dimensional position-sensitive detector and is used to investigate relatively large structures (up to ~500 Å) in metallurgical, polymer, chemical, and biological systems. A diversity of materials such as Portland cement, coal, collagen, alkoxide-derived sols, and Fe-Cr alloys have been studied on this instrument. An important capability of SAD is its large dynamic Q-range, which results from the use of the time-of-flight method and permits collection of data from 0.005 Å<sup>-1</sup> to 0.35

$\text{\AA}^{-1}$  in a single experiment with a single instrument setting. A variety of ancillary equipment is now available for use with SAD, including furnaces (up to 1900 K), closed-cycle refrigerator (down to 15 K), ambient-temperature sample changer, and a magnet (10 kG).

The broad scientific interest in the SAD and its consequently large oversubscription have resulted in the decision to build a second small angle diffractometer with expanded capabilities, and this instrument (SAND) is currently being installed at IPNS. After a suitable commissioning period, SAND is expected to become the primary small-angle scattering instrument available to the IPNS user program, at which time SAD will be taken out of service and possibly rebuilt. SAD was one of the pioneering time-of-flight, small-angle scattering instruments in the world, and the design of SAND has been able to benefit from the enormous amount of development and refinement which has taken place on SAD during its many years of operation. SAND will have two automatically interchangeable sets of converging multiple-aperture collimators, so it can operate in either a low-resolution mode or a high-resolution mode to allow optimal trade-off between Q-range and intensity for a given experiment. It also has a cooled MgO filter in the incident beam to remove most of the fast neutrons and views the same solid methane moderator viewed by SAD. A chopper is provided to eliminate most of the background caused by delayed neutrons. A  $40 \times 40\text{-cm}^2$  area detector covers the forward scattering angles while a bank of 65 linear-position-sensitive detectors (LPSDs) (total active area  $\sim 60 \times 70\text{ cm}^2$ ) covers higher angles. The bank of LPSDs extends the maximum scattering angle up to  $36^\circ$ , making a huge improvement in the counting statistics in the higher-Q portion of the data and allowing SAND to cover an extremely wide Q-range with one setting. The Q-range extends up to  $0.4\text{ \AA}^{-1}$  even when wavelengths are restricted to  $\lambda > 5\text{ \AA}$  (above the Bragg cutoff for most crystalline samples), and much higher when the full wavelength range down to  $\lambda = 1\text{ \AA}$  can be used. The short flight path of the instrument (9 m source-to-detector) permits the use of wavelengths up to  $14\text{ \AA}$ , and the use of the  $\sim 20\text{ K}$  solid methane moderator ensures a reasonable cold neutron flux even at this wavelength. Only one set of collimators is presently available, and with this set the practical  $Q_{\min}$  is  $\sim 0.005\text{ \AA}^{-1}$ . Later a second set of multiple-aperture converging collimators with tighter collimation will become available, and then  $Q_{\min}$  and Q-resolution down to  $\sim 0.002\text{ \AA}^{-1}$  will be possible.

The Polarized Neutron Reflectometer (POSY)<sup>6</sup> utilizes polarized neutrons and the neutron reflectometer techniques developed at IPNS for obtaining magnetization density information in thin films or near the surface of bulk materials. The very interesting basic information is coupled with some promising applied interest, for example magnetic hysteresis in materials for recording heads. Because this technique (with unpolarized neutrons) was also found to have a wide variety of applications in the study of chemical density profiles in polymer and other thin films, a second reflectometer (POSY-II)<sup>7</sup> was constructed as a PRT instrument with the financial assistance of IBM. This unpolarized version of POSY shares a beam port with POSY, but is a fully independent instrument which is used primarily for studies of interfaces and interdiffusion in polymers, taking advantage of the large scattering contrast of H and D.

The two chopper spectrometers (LRMECS - Low Resolution Medium Energy Chopper Spectrometer, HRMECS - High Resolution Medium Energy Chopper Spectrometer<sup>8</sup>) are very general inelastic scattering instruments equipped with detectors spanning angles between  $2^\circ$  and  $120^\circ$  and utilizing incident beam energies from 2 meV to 2 eV. These have been the workhorses of the IPNS inelastic scattering program and have proved exceptionally versatile in a variety of problems involving measurements of the inelastic scattering function  $S(Q,E)$ . Experiments on electronic transitions, vibrational spectroscopy of amorphous and crystalline systems, and momentum distributions have all made use of the abundant epithermal spectrum available at IPNS. Many measurements made on the chopper spectrometers are not generally accessible at steady-state sources because beam intensities fall off sharply for energies above  $\sim 100$  meV. Recently these instruments have proven very useful at low energies, with spectroscopy having been done with incident energies as low as 1.9 meV.

Because of the very heavy demand for beam time on the chopper spectrometers by the groups involved in momentum density measurements in quantum liquids and solids, a new chopper spectrometer (PHOENIX), designed only for high-angle inelastic scattering using epithermal neutrons, was built and installed as a PRT effort. This instrument is dedicated

primarily to the momentum density measurements. A large dilution refrigerator for cooling the samples as low as 0.3 K is an integral part of this instrument. A second detector bank has recently been installed at smaller scattering angles in order to provide limited capability for diffraction measurements for *in situ* sample characterization.

The Quasielastic Neutron Scattering Spectrometer (QENS)<sup>9</sup> is optimized for quasielastic scattering measurements, but is also quite useful used for chemical spectroscopy in the 0-50 meV energy transfer region. It takes advantage of good energy resolution (70  $\mu$ eV at zero energy transfer), coupled with the ability to measure energy changes as a function of momentum transfer. Three variable-angle analyzer-detector packages select a scattered energy of ~3.6 meV and enable scanning of scattering angles between 25° and 120°. QENS was also built and is operated as a PRT instrument, with the major programs of study including dynamics and diffusion of ions and adsorbed molecules in molecular sieves, zeolites, clays, and intercalates; dynamics of supercooled water; dynamics of hydrocarbons; and dynamics of biological molecules.

In addition to the data acquisition systems for the instruments, IPNS also provides a central computer cluster for data analysis, and on this cluster the instrument scientists maintain the extensive suites of analysis codes necessary for complete data reduction and analysis for most types of experiments. Major packages include the Rietveld profile refinement codes for powder diffraction data (including provisions for handling multiple phases, texture, anharmonicity, geometrical shape constraints, strain broadening, and amorphous components), codes for multiplet peak fitting of powder diffraction data, a suite of analysis software for structural data in amorphous systems (including corrections for multiple scattering and inelasticity), codes for quantitative analysis and presentation of texture data, codes for reduction and presentation of single-crystal diffraction data and for structural determinations using such data, a full suite of codes for reduction and analysis of small angle diffraction data, codes for modeling reflectometer data, and an extensive set of reduction and analysis codes for chopper instrument data (including multiple scattering and multiphonon corrections). All users are welcome to complete at least the first stages of their data analyses using these facilities, and first-time users are strongly urged to do so since then they can benefit from the experience of the local staff. Most of the analysis packages are fairly portable, so many of the repeat users have also installed the relevant codes at their own facilities.

Additional information on IPNS instruments is available on the World Wide Web. The IPNS World Wide Web Server can be accessed by opening the following Uniform Resource Locator (URL) from within Mosaic: <http://pnsjph.pns.anl.gov/ipns.htm>

## B. INSTRUMENTATION POSSIBILITIES FOR THE IPNS UPGRADE, A 1-MW SPALLATION SOURCE

The potential for significant increases in the near future in neutron scattering capabilities at pulsed spallation neutron sources (PSS) is great. A 1 MW PSS would represent a factor of 6 gain over the present level of ISIS (UK), the world's most powerful spallation neutron source, which has operated since 1985. A source with an increase by another factor of 5 is being proposed for the European Spallation Source (ESS). In addition, there is significant potential for future enhancements in advanced spallation sources since there are no fundamental limitations for even further improvements in the technology. In addition to being the most powerful pulsed source in the world, a 1-MW PSS would also act as a test bed for concepts for more intense sources in the future. The complementary nature of pulsed and steady state neutron sources argues strongly for developing advanced pulsed source capabilities in addition to advanced reactors, such as the ANS. This was one of the major recommendations of the BESAC Panel on Neutron Sources (1992) chaired by W. Kohn.

A feasibility study of a new 1 MW pulsed neutron source, the IPNS Upgrade, has recently been completed. (Full details of this feasibility study have been published as an Argonne Report and as part of the Proceedings of the International Collaboration on Neutron Sources-XII, May, 1993.) The source will consist of a 400 MeV Linac injecting 500 microamps of protons into a Rapid Cycling Synchrotron, which accelerates to a final energy of 2.0 GeV (a

nominal beam power of 1 MW). The beam will be delivered to two target stations at 10 and 30 Hz. Six moderators on each target (water, liquid hydrogen or liquid methane) will provide 36 neutron scattering beam ports, radiation effects facilities in both targets, rabbit tube irradiation and activation facilities; and other capabilities are being considered. The IPNS Upgrade would require 4-5 years from the design decision to completion and would be site specific and use existing Argonne infrastructure (buildings, water and electrical systems, shielding, etc.) which will result in a cost savings of more than \$100M. The total project cost is estimated to be on the order of \$500M. As part of the design process, joint workshops were held with Los Alamos on Accelerators for Future Spallation Neutron Sources in Santa Fe on February 16-20, 1993, and on Technological and Scientific Opportunities at a 1-MW Pulsed Spallation Neutron Source at Argonne on May 13-16, 1993.

The decision on the repetition frequency of the accelerator for the IPNS Upgrade was based on the optimal frequency for the neutron scattering instruments. A survey of opportunities and an evaluation of preliminary designs for neutron scattering instruments for a 1 MW pulsed source led to a table of the various requirements that they place on the neutron source, which have fundamentally affected the definition of the project. A repetition frequency of 30 Hz was found to be clearly preferable to 60 Hz.

Two roughly equally populated categories of instruments emerged from the study of scattering instruments, those for which 30-Hz pulsing (but not much higher) is satisfactory, and those which require lower frequency of pulsing and for which 10 Hz is satisfactory. Serving these two categories of instruments led to the requirement of two separate targets. The total number of instruments and correspondingly the number of neutron beams and, in addition, the number of differently optimized moderators needed exceed the number that can be arranged around a single shielded target station; and this also spells the need for two target stations to provide for the required number of moderators and beams. Therefore the accelerator delivers one out of three pulses to a low frequency station at 10 Hz, the high frequency station normally receiving the remainder of the 30-Hz pulse train in iambic pattern.

The IPNS Upgrade will provide 36 beam ports for neutron scattering instruments, 18 each at the 30-Hz and 10-Hz target stations. Neutron beams for more than one instrument will be extracted from a single beam port in some cases, so more than 36 neutron scattering instruments can be supported at this facility. There will be a total of 12 moderators, one for every three beam ports, so the moderator characteristics can be optimized to the requirements of the individual instruments. A representative set of 27 instruments that would occupy 24 of the beam ports and would provide a well-balanced initial instrumentation complement is given below. The remaining 12 uninstrumented beam ports will be available for later development and installation of new state-of-the-art instruments, as well as for the installation of specialized instruments developed by Participating Research Teams (PRT's).

This representative set of instruments has been used in selection of the target station parameters, in laying out the locations of the target stations within the experimental halls, and in providing the cost estimates. **This is certainly not the exact set of instruments that will be built, and considerably more input from the user community will be solicited before deciding on the actual instrument complement to be included as part of the project.** It is anticipated that up to 10 instruments that are currently operating at IPNS would be refurbished and transferred to the IPNS Upgrade as part of this initial instrument complement. This will provide a core of proven instruments ready for operation on day one. The neutron scattering instruments will be located in existing experimental halls, which can provide internal space for beamlines up to 50 m long (see Figure 3). Beamlines can easily be extended outside the buildings if necessary, since much of the external space is parking lots.

Most of the neutron scattering instruments will use the neutron time-of-flight (TOF) principle for determination of neutron wavelengths. Of these, the majority require good wavelength resolution, and for such instruments the IPNS Upgrade target stations will provide roughly 50 times the intensity available at IPNS. However, for those instruments which do not require good wavelength resolution, for example small-angle-scattering instruments, the moderators can be optimized to provide roughly 200 times the intensity available at IPNS.

However, the IPNS Upgrade will be sufficiently intense that it will no longer be necessary that all instruments be based on TOF techniques. With moderators optimized for total neutron output rather than for sharp neutron pulse structure, time-averaged thermal or cold neutron

fluxes will be equivalent to those at a medium flux reactor. (A cold neutron flux of  $7 \times 10^{13}$  n/cm<sup>2</sup>/s has been calculated for one of the liquid hydrogen moderators at the IPNS Upgrade.) Thus, any instrument that would work at a medium-flux reactor can be made to work at least as well at the IPNS Upgrade. Furthermore, even a moderator optimized for high time-averaged flux will have a pulse width of less than one millisecond, and so will have a duty factor of 1:30 or less. This time structure can be used to significant advantage even on nominally steady-state instruments to reduce background, eliminate unwanted orders from crystal monochromators, etc. A cold-neutron triple-axis spectrometer operating in this "quasi-steady-state" (QSS) mode is proposed as one of the initial complement of the IPNS Upgrade instruments, and several other types of QSS instruments are under consideration which might have unique advantages for particular types of experiments.

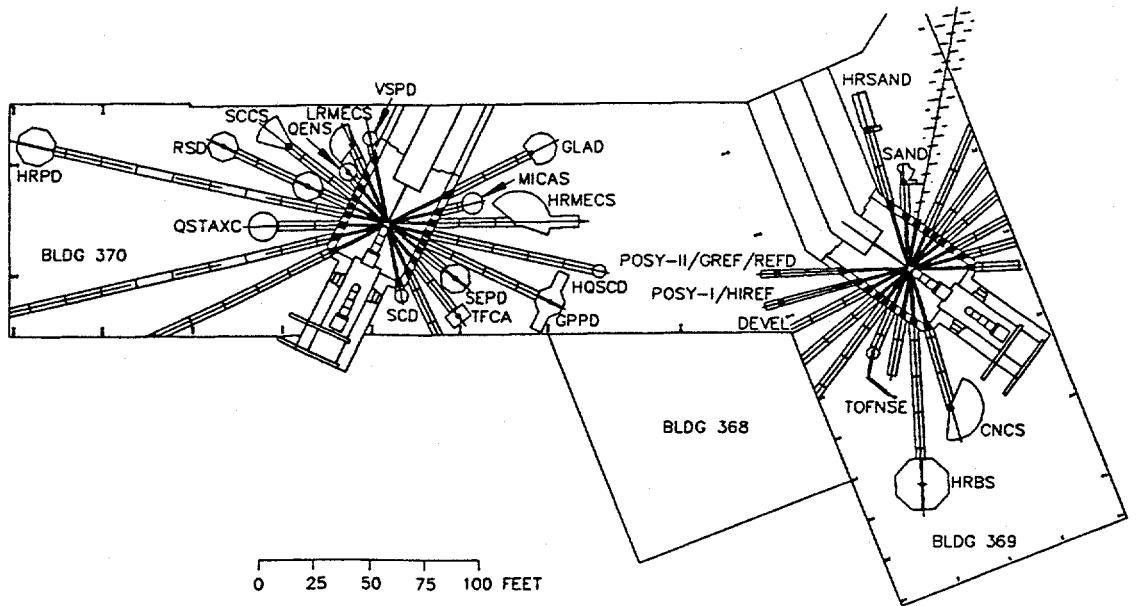


Figure 3. Location of the reference set of instruments on the neutron beamlines.

Although the primary function of the IPNS Upgrade is neutron scattering, the facility can provide many other types of capabilities as well. Some of these, such as neutron radiography, could utilize one or more of the neutron beam ports. Although no such use is included among the instrumentation for the first 24 beam ports, the feasibility study will discuss several potential uses of this type. In addition, the IPNS Upgrade is well suited to the performance of neutron irradiations for radiation damage studies, isotope production, and neutron activation analysis. Facilities for these purposes are included as part of the IPNS Upgrade project. Space is available for other experimental facilities not included in the scope of the project, such as pulsed muon spin rotation, nuclear physics, neutrino physics and medical isotope production.

Table III lists the 15 diffractometers and reflectometers in the reference set, and indicates their expected performance based on these source parameters. The five powder diffractometers are variously optimized for small samples (10-100 mg), high intensity, high resolution at 90° (0.2% in  $\Delta d/d$ ), high resolution (0.08% in  $\Delta d/d$ ), and for residual stress measurements on various types of samples. The general purpose small-angle diffractometer has an extremely broad dynamic range in  $Q$ , and it is complemented by a high-resolution instrument ( $Q_{\min} = 0.0005 \text{ \AA}^{-1}$ ) and by an instrument which can be reconfigured for various types of specialized small-angle scattering experiments (such as resonance small-angle scattering, measurements of inelastic effects, etc.). Additional diffractometers include a diffractometer for amorphous materials, and two single-crystal diffractometers, one of which is optimized for high real-space resolution (measurements made at  $Q$  values up to  $30 \text{ \AA}^{-1}$ ).

The suite of four reflectometers plus one reflectometer development beam is clustered on two beam ports, since the reflectometers are small and require only very narrow beams. This

suite includes a polarized-neutron reflectometer, a general purpose reflectometer, a high-intensity reflectometer (reflectivities down to  $10^{-4}$  in 1 min), and a reflectometer optimized for measurement of off-specular scattering. The latter three instruments have horizontal sample geometries, so that liquid samples can be accommodated.

Table IV indicates the expected performance of the 10 remaining instruments, which are designed for inelastic scattering measurements. There are four chopper spectrometers including an instrument optimized for work with cold neutrons (better resolution but slightly lower intensity than IN5 at ILL) and one optimized for the study of excitations in single crystals, as well as traditional general-purpose instruments in both low and high resolution versions. Included among the five crystal analyzer spectrometers is the cold-neutron triple-axis spectrometer which operates in a quasi-steady-state mode as discussed above. The other four crystal analyzer spectrometers are time-of-flight instruments. Two of these are optimized for medium resolution ( $70 \mu\text{eV}$ ) and high resolution ( $1-5 \mu\text{eV}$ ) measurements at low energies, one is optimized for relatively high resolution chemical spectroscopy at high energies, and one is a multi-angle spectrometer for the study of excitations in single crystals. The final instrument intended for inelastic scattering measurements is a spin-echo spectrometer. This instrument utilizes cylindrical field geometry, and is the time-of-flight counterpart to IN11 at ILL. Resolution is expected to be better than at IN11, while data rates are expected to be somewhat lower than at IN11.

Table III—Reference Set of Diffractometers and Reflectometers at the IPNS Upgrade

Powder Diffractometers		Range for d (Å)	Best $\Delta d/d$ (%)	Measurement Time (min)
VSPD	very small samples (10-100 mg)	0.2-17	0.35	70
SEPD <sup>a</sup>	high intensity	0.2-17	0.35	3
GPPD <sup>b</sup>	medium resolution (excellent at 90°)	0.2-9	0.2	10-60
HRPD	high resolution	0.2-5	0.08	50
RSD	residual stress (12-m position)	0.3-6	0.55	50
	(25-m position)	0.2-3	0.30	10
Small-Angle Diffractometers		$Q_{\min}$ (Å <sup>-1</sup> )	$Q_{\max}$ (Å <sup>-1</sup> )	Measurement Time (min)
SAND <sup>a</sup>	general purpose (wide Q range)	0.002	2	1-90
HRSAND	high resolution	0.0005	0.4	60-1800
SPSAND	reconfigurable for special purposes	----- variable -----		
Amorphous Materials Diffractometer		Range for $Q$ (Å <sup>-1</sup> )	$\Delta Q/Q$ (%)	Measurement Time (min)
GLAD <sup>a</sup>	liquids and glasses	0.07-120	1.2-10	10-50
Single-Crystal Diffractometers		Range for $Q$ (Å <sup>-1</sup> )	$\Delta Q/Q$ (%)	Measurement Time (min)
SCD <sup>a</sup>	general purpose	0.9-17	0.6-0.9	20-200
HQSCD	high real-space resolution	2-30	0.4	~200
Reflectometers		Sample	Minimum Reflect.	Measurement Time (min)
POSY-I <sup>b</sup>	polarized neutrons	vertical	$10^{-6}$	60-120
POSY-II <sup>b</sup>	general purpose	horizontal	$10^{-7}$	60-120
HIREF	high intensity	horizontal	$10^{-4}$	< 1
GREF	grazing incidence	horizontal	$10^{-7}$	60-120

<sup>a</sup> Transferred from IPNS with little change.

<sup>b</sup> Transferred from IPNS with some modification

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**Table IV—Reference Set of Inelastic Scattering Instruments at the IPNS Upgrade**

<b>Chopper Spectrometers</b>	Range for $E_{inc}$ (meV)	$\Delta E/E_i$ (%)	Measurement Time (h)
HRMECS <sup>b</sup> high-resolution general purpose	4-2000	2-4	2
LRMECS <sup>a</sup> low-resolution general purpose	3-2000	4-7	<1
CNCS high-resolution low energy	0.3-20	<1	12
SCCS excitations in single crystals	50-2000	~1	~12
<b>Crystal-Analyzer Spectrometers</b>	Range for $E$ (meV)	$\Delta E$ (meV)	Measurement Time (min)
TFCA general purpose	0-1000	0.5-30	20-80
QENS <sup>a</sup> quasielastic, medium resolution	0-150	0.05-3	20-80
HRBS microvolt resolution	0-10	0.005-0.06	~80
MICAS survey of single-crystal excitations	0-20	varies	
QSTAXC cold-neutron triple axis (QSS)			
<b>Spin-Echo Spectrometer</b>	Spectral Resolution (meV)	$\Delta Q/Q$ (%)	Measurement Time (h)
TOFNSE TOF spin-echo, cylindrical geometry	$10^{-6}$ - $10^{-1}$	1.5	2-48

<sup>a</sup>Transferred from IPNS with little change

<sup>b</sup>Transferred from IPNS with some modification

QSS Quasi-steady-state

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