

INSTRUMENT DEVELOPMENT FOR MATERIALS SCIENCE RESEARCH AT WNR

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I. INTRODUCTION

The neutron scattering program at the Los Alamos spallation neutron source is based on the operational WNR facility which provides up to 11 μA of 800 MeV protons to a target in pulse widths up to 8 μs at 120 Hz. The immediate goals of the program are:

- to gain experience with neutron instrumentation at spallation neutron sources;
- to explore the scientific potential for condensed matter research at these sources.

The proton storage ring (PSR) funded for construction will provide 100 μA in 0.27 μs pulses at 12 Hz, therefore greatly improving intensity, time-of-flight (TOF) resolution, and repetition rate. The longer term program goal is to develop a condensed matter research and instrument capability to make optimal use of the PSR when it becomes operational in 1985.

The initial emphasis, given limited manpower and resources, has been placed on developing a set of prototype instruments which are relatively easy to implement and which take advantage of the unique characteristics of the present WNR when compared with reactor neutron sources. Given the advantage of a working spallation source, we can test instrument developments as we proceed. In instrument development we have addressed problems common to all spallation sources, e.g. shielding against fast neutrons, chopper phasing to the variable line frequency, electronics for multidetector arrays, megaword memories for position sensitive detectors, and slab vs wing geometry moderators. These developments are closely coupled to the experimental optimization of targets and moderators reported by G. Russell at this meeting.

The instruments currently being developed at the WNR (see Fig. 1) are:

- a crystal analyzer spectrometer and a filter detector spectrometer on the same beamline for inelastic scattering
- a chopper spectrometer
- an electronic time and resolution focused general purpose diffractometer for powder, liquid, and amorphous samples
- a geometrically time focused special environment diffractometer for powder diffraction
- a single crystal diffractometer based on the LAUE TOF technique

II. FACILITY DEVELOPMENTS

The WNR has a vertical injection target with 12 neutron beam tubes viewing the target/moderator assembly. All the experiments reported below used Cd poisoned 1/2" polyethylene moderators. The initial experiments used a hybrid slab water moderator with some beam tubes viewing the target and some offset. For the most recent experiments, a new reflected T-shaped target/moderator assembly is used with all neutron beam tubes in offset geometry. This has greatly improved signal-to-noise as illustrated below.

We have also constructed new liquid Hg beam shutters. These use lead inner collimation to block the view of the target, a Hg vessel in the center operated by a He pressure system, and interchangeable outer collimators adapted to the individual instruments. These shutters have proven to be effective and to be inexpensive (\$12 K/each) to construct. For the present experiments background caused by the scattering of neutrons from the inner surfaces of the shutter has not been a problem.

Behind each instrument an evacuated get-lost-pipe carries neutrons to a beam dump placed in the recesses in the walls of the experimental hall, or outside the hall where possible. In a beam dump, fast neutrons reflected back from the walls will see first Pb bricks, then polyethylene, Cd sheet, and finally concrete bricks. The radiation levels at the beam dumps have been high, indicating that a future optimization is required.

All the experiments described below were carried out with $\sim 3 \mu\text{s}$ proton pulse widths and less than 3 μA on target. We have not realized the

WNR potential for neutron flux-hours due to various difficulties. Among these are fast kicker magnet reliability, the splitting of available beam time with nuclear physics research, LAMPF operation in a variable energy mode in the most recent cycles, and the use of nonoptimized target/moderator assemblies. We expect significant improvements in these operational problems in the near future.

III. INELASTIC NEUTRON SCATTERING SPECTROMETERS

A. Crystal Analyzer Spectrometer (CAS)

A prototype crystal analyzer was installed at flight path 5 in July 1979 at which time the target was viewed directly by the beam tube. The instrument utilized a set of nonoptimal pyrolytic graphite crystals with a mosaic spread of 0.4° . Four of those crystals of dimension 5 cm wide by 7.5 cm high were mounted in a time-focused geometry with a mean scattering angle $2\theta_A = 90^\circ$ at an angle of 90° and a distance of 50 cm from the sample. A Monte Carlo computer code due to Sköld (Crawford, private communication) was used to optimize the crystal and detector geometries. Two blocks of beryllium, each with a cross-sectional area of $10 \times 10 \text{ cm}^2$ and length of 20 cm, separated by a cadmium sheet, were placed between the analyzer crystals and the detectors for elimination of higher orders. Thus the instrument had a final flight path of 1 m with a source-sample distance of 5.65 m. The incident beam was approximately 7.5 cm high and 4 cm wide.

Spectra obtained with the prototype instrument included those of TiH_2 , ZrH_2 , and NaHF_2 . The noteworthy points of these trial runs were:

- the good energy resolution of the instrument: e.g. the splitting of the TiH_2 fundamental optic peak was easily observed
- the background at early times (energy transfer greater than 100 meV) was large and rising steeply but was low in the thermal region
- cooling the filter was necessary

The crystal analyzer was then moved to the tangential flight path 6 as well as improved in several other ways. The analyzer crystal array was enlarged to include six of the 0.4° mosaic graphite crystals, more suitable ^3He counters were used in the counter bank, and a liquid nitrogen cryostat was installed to cool the beryllium filter. The present graphite analyzer

incorporates further improvements, primarily in shielding. A view of the crystal analyzer combined with the separate prototype beryllium filter detector (see below) is shown in Fig. 2. The large improvement in background, which we attribute to the move to a tangential flight path, is demonstrated by the TiH_2 spectra shown in Fig. 3. In the present configuration the background counting rate in the crystal analyzer is approximately 1/4 count per 3.2 μs channel per hour in the thermal neutron region, and approximately twice that amount in the epithermal range.

At present the graphite crystal analyzer is considered to be operating in a production mode even though the instrument is not quite optimized. Installation of graphite crystals of approximately 1.2° mosaic of a size large enough (10 cm high) to accept the total beam would almost double the count rate with no deterioration of the energy resolution. This modification is being considered for the near future since in the present configuration a typical metal hydride spectrum takes approximately 24 hrs. to acquire with satisfactory counting statistics.

Extensive data has been collected on $\text{NbH}_{.87}$ at four different temperatures between 10 and 300 K. Some of the results are shown in Fig. 4 from which it was found that the hydrogen local mode peaks become split at temperatures somewhere below 200 K. At 78 K the magnitude of the splitting obtained by fitting Lorentzians convoluted with a Gaussian for the instrumental resolution is 8.4 meV at an energy transfer of 120 meV for which the calculated energy resolution is 5.5 meV FWHM. The intrinsic width of the peaks was found to be 1.5 meV, thereby indicating that the energy resolution of the instrument is known quite accurately. Additional evidence to support this conclusion is given by the fact that the results at 300 K agree very well with those of Richter and Shapiro as obtained at a Brookhaven High Flux Beam Reactor. The deuterides did not show the same effect.

A principal aim of the work on NbH is to gain information on anharmonic effects on the local hydrogen potential. To this end efforts were made to discern the higher harmonics of the local modes. However, because of the additional complication of the splitting in the low-temperature spectra, the weak peaks at higher energy transfers cannot be unambiguously identified, while in the high-temperature spectra the peaks are broadened too much. A sample with a concentration of 78% H which in a previous measurement was found not to have undergone the same transformation as in the 87% sample is currently being investigated for the purpose of measuring the higher harmonics.

Several options are being considered for the future development of the crystal analyzer. Initially, we would like to improve energy resolution at large energy transfers. For this purpose the construction of a time-focused Ge(111) arm is being studied with a final energy of about 50 meV (Fig. 5). A trial setup for the investigation of count rates and background problems will use a Ge(111) crystal of large mosaic ($\sim 1^\circ$) previously used by Day and Sinclair. In preparation for the much higher intensity neutron beams available when the PSR comes on line, crystal analyzers for single crystal work such as the "constant Q" and "high symmetry" instruments will be investigated.

B. Filter Detector Spectrometers (FDS)

As part of the initial crystal analyzer trials a simple beryllium filter instrument was first set up at the target-center-looking flight path 5,5.65 m from the source, with a sample to detector distance of 45 cm. Two $10 \times 10 \text{ cm}^2 \times 20 \text{ cm}$ long Be blocks were used uncooled. After the move to flight path 6 the filter detector was mounted opposite the crystal analyzer (Fig. 2) for a more direct comparison between the two instruments. The principal trade-off between the two instruments was a count rate more than a factor of 50 greater for the FDS than the crystal analyzer but a factor of three degradation in resolution. Experience with these prototypes indicates that both may be of use.

Since for large energy transfer the resolution of the FDS depends crucially on the ratio of final to initial flight paths, the present instrument was installed at a second sample position 11.42 m from the source and "downstream" from the crystal analyzer. In addition, five new Be pie sections were fabricated, each 10 cm high with an inner radius of about 9 cm radial length of 15 cm and subtending 18° of scattering angle. The individual wedges are separated by Cadmium foil and each section is individually time-analyzed by six $1/2$ " diam, 10 atm ^3He counters. The final flight path is 28 cm and its dimensions were largely determined by requirements for sample cryostat and future filter cryostat dimensions along with a minimum thickness of filter material.

The much improved resolution and background characteristics of this new filter instrument became quite obvious in the comparison shown in Fig. 6 which shows raw data on ZrH_2 . The spectrum from the present FDS is that of one of the pie sections only. The energy resolution of this instrument has improved to about 10% ($\Delta E/E$, FWHM) with data rates still higher than the crystal

analyzer in spite of the fact that the filter is not yet cooled. A more recent set of data is shown in Fig. 7 on the temperature dependence of the $\text{FeTiH}_{1.14}$ (β -phase) local mode spectrum.

Since the inelastic neutron scattering program at WNR includes studies where sample size may become a problem, the FDS will be retained. A liquid-nitrogen cooled Be/BeO difference filter as shown in Fig. 8 is under construction. The final flight path will remain about 28 cm while the initial flight path (currently 11.42 m) may be increased to about 15 m by moving the instrument to a flight path of its own (flight path 7).

C. Chopper Spectrometer (CS)

The initial effort on inelastic neutron scattering at the WNR centered on a high energy transfer, small-Q chopper spectrometer. The 240 Hz Fermi chopper with Cd slits, a low-angle detector bank, and associated shielding were acquired from the MTR in Idaho. The chopper was installed 5 m from the source and 50 cm in front of the sample. The evacuated final flight path was 2 m and contained 24 $1''$ ^3He counters at an average scattering angle of 5° . No additional shielding or collimation were constructed.

The primary purpose of these experiments was to learn how to phase the neutron chopper with the LAMPF proton pulses. Since the proton pulses are fired at the crossing, t_0 , of the line voltage from the power grid, the frequency and phase of the proton pulses are variable. The period can vary by as much as 2 μs on a 10 s time scale resulting in phase errors of several milliseconds. We have developed a technique to define the phase to within + 1 μs , for a range of 16 values spaced 64 μs apart, but the method is limited as we shall discuss. The importance of the ability to control the timing of beam extraction cannot be overemphasized. This will be possible at the WNR when the proton storage ring becomes operational.

The WNR chopper operates by: (1) controlling the period and phase of the chopper using a microprocessor based active damping system, and (2) by selecting the time of firing the LAMPF proton pulse within an allowed window of 64 μs about the LAMPF t_0 . The microprocessor averages the period error over a full libration period, and makes a correction of 80% of the computed value of the maximum acceleration. This simple feedback system is adequate to maintain the long term average rotor period within a fraction of 1 μs of the accelerator.

The phase of the chopper cannot be tightly defined because of the rotor stability, and the time required for feedback control. As a result the control system can only achieve a distribution of phase errors, typically with a FWHM at 400 μ s centered about the correct phase, i.e., the desired incident neutron energy. To fire the LAMPF proton beam, a train of 16 pulses, produced 64 μ s apart, is sent to LAMPF and a measurement of the chopper phase relative to the succeeding t_0 tells which (if any) of the pulses fell into the allowed window, and therefore fired the proton beam. Data collected from that neutron pulse is sorted into one of 16 different spectra each corresponding to a different incident energy. In the most recent operation of the chopper spectrometer, typically about 90% of the data fell into eight different spectra with about 30% of neutrons at the nominal incident energy. A schematic of the control system is shown in Fig. 9. Fig. 10 shows the spectra of TiH_2 taken at two incident energies with this method. The peak at ~ 140 meV is apparent in both spectra.

While this control scheme is adequate, data collection is for several incident energies simultaneously so that the signal-to-noise at any given spectrum is reduced. Also, this method will work for only one chopper at a time. Recently, LAMPF operations has agreed to widen the window to 128 μ s which will improve signal-to-noise somewhat. The data in Fig. 10 also show a large background due to inadequate shielding against neutrons scattered by the chopper. The MTR chopper is unsuitable for scientific research at the WNR because of its poor mechanical reliability, and because it has a Cd slit package which is ineffective for epithermal neutrons. The next step is to acquire a chopper with a boron slit package, to build proper shielding and collimation, and to optimize further the control system. At present, this has been postponed because of budgetary and manpower limitations. Chopper development will have high priority in the planning for instruments to be available when the PSR becomes operational, at which time phasing will not be a problem.

IV. DIFFRACTION INSTRUMENTS

A. The General Purpose Neutron Diffractometer (GPD)

A time-of-flight neutron diffractometer has been built at the WNR pulsed source with a capability for liquid, amorphous, and medium resolution powder diffraction ($0.5\% \Delta d/d$) experiments. The instrument tests the concepts of electronic time and geometric resolution focusing. The instrument consists of

62 3He proportional counters arranged in four banks at scattering angles 150° , 90° , 40° , and 10° , and two ^{235}U fission beam monitors. Each bank of detectors is mounted inside a borated polyethylene box and nose cone, designed to eliminate as much background scattering as possible. The whole detector array and sample position are housed in a shielded room constructed from large slabs of borated wax 30 cm thick contained in steel plate. This modular design will facilitate future modifications. See Fig. 11.

The sample is located 10 m from the target and the detectors are located 1 m from the sample, except for the low-angle bank where the flight path varies from 1 m to 2 m. The detector banks are angled relative to the scattered beam: this is the so-called resolution focussed configuration, where each detector in a bank has approximately the same resolution. The nominal specifications for each bank are shown in Table I.

Scattering Angle (2θ)	No. of Detector	Detector Height (cm)	Sample-Detector Path Length (m)	Resolution [$\Delta d/d(\%)$]*
10	14	15 and 30	1-2	8-12
40	16	15	1.0	2
90	16	30	1.0	0.8
150	16	30	1.0	0.5

*at $\lambda \sim 1.3 \text{ \AA}$

The incident collimator consists of an evacuated aluminum pipe with poly-boron inserts (5% boron) throughout its length. The area of the moderator viewed is 10 cm high by 5 cm wide and the collimator tapers this in five stages to a beam 5 cm high and 1.3 cm wide at the sample position. The walls of the collimator are smooth and uncoated. This configuration has produced a cleanly defined beam at the sample position with little spreading.

After the sample the beam passes through a box filled with argon, to reduce air scattering into the low-angle bank, and then into an evacuated get-lost-pipe which carries the beam a further 10 m to a beam dump outside the experimental room. The well-defined character of the beam can be seen from the fact that an "Albatross" neutron monitor placed on the get-lost-pipe

registered about 3 mR/hr but when placed near the beam dump recorded 120 mR/hr. So far we have not been able to test for beam carried background (i.e., neutrons down-scattered by the collimator and arriving at the sample at later times.)

A schematic for the electronics to accumulate neutron counts is shown in Fig. 12. The output from each detector is fed into a Le Croy charge sensitive pre-amp TRA510. The output of the pre-amp is pulse shaped to have a width of ~ 250 ns and this narrow width is partly responsible for its low amplitude (~ 4 mV). The outputs from all the pre-amps are fed into a multiplexer by co-axial cables which vary in length from 0.5 m to 2 m. The signals are amplified and discriminated using a Le Croy Model PC 700 hybrid, and then multiplexed for subsequent computer processing. The discriminator level is set for 32 detectors by one control.

We have found this system susceptible to the r.f. noise present in an accelerator environment. We believe we are susceptible to this noise primarily because of the low level signal from the preamplifier. Other problems have arisen from having one discriminator control for many detectors. We are presently considering both a reconfiguration, which should overcome the major problems, and alternative preamp/amplifier/discriminator systems which can be purchased at reasonable cost. There have been no problems with multiplexing 64 detectors into the CAMAC crate.

Experimental Data: Preliminary samples have been run to characterize the instrument. Figure 13 shows the raw data from 16 detectors combined as they would be for a powder diffraction experiment, for a vanadium rod 0.635 cm in diameter and 5 cm high, together with the air scatter over an equivalent counting period. The vanadium count rate suggests a thermal flux at the sample of $\sim 1 \times 10^5$ n/cm²-s. The relatively low background is a source for encouragement. Fig. 14 shows part of a MgO powder pattern for the 150° bank of detectors, taken in about seven hours. In Fig. 15 we show a preliminary analysis of a diffraction experiment on D₂O, compared to a typical reactor spectrum. No absorption, multiple scattering or Placzek corrections have been made, but the measured spectra have been divided by the incident beam monitor and then normalized to the vanadium data to remove the counter efficiencies. It will be seen that the structure factor possesses all the usual features for D₂O. The Placzek 'droop' which appears in reactor data has largely disappeared, even for a material for which $S(Q, \omega)$ is quite broad in ω relative to thermal energies.

Future Program: Initially we expect to use the instrument on a variety of simple experiments: crystalline powders particularly to look at magnetic structures at large d-spacings; molecular liquids and gases, to determine the variation of bond lengths as a function of pressure and temperature, and also determine inter-molecular orientations; structures of amorphous materials, where a broad range of momentum transfers are required. For accurate work it will probably prove necessary to incorporate a frame overlap chopper which is at a design stage.

B. Single Crystal Diffractometer (SXD)

A diffractometer is under development at the WNR for single-crystal structure determinations and the study of diffuse and incoherent scattering. The design is similar to an instrument being developed at ANL, but it has some unique features such as a novel megaword memory data acquisition system.

The heart of the single crystal instrument is a 2 atm ³He filled multiwire Borkowski-Kopp type position sensitive area detector with dimensions 25 cm x 25 cm procured from Technology for Energy Corporation in Knoxville, Tennessee. This detector is designed to acquire data from a volume element consisting of x-y spatial information with a resolution of 2mm and time-of-flight information with a wavelength dependent resolution. This detector is mounted on a portable frame and is positionable at several distances and orientations from the crystal. A schematic of the instrument is shown in Fig. 16. The crystal is positioned in the beam with a quarter circle goniostat. The Hg filled shutter collimation system views a 10 cm x 10 cm area of the moderator and a 0.5 cm x 0.5 cm area of the sample. The moderator to sample distance has been chosen to be 5.8 m, just outside the biological shield, to attain the maximum neutron flux.

We have attempted to keep the geometrical features of the instrument as simple as possible in the initial design to maintain flexibility. Among the features which we plan to develop and include in the instrument are a more sophisticated automated goniostat, continuously variable detector positioning, and variable temperature and pressure sample environments.

Data Acquisition: The area detector design includes two orthogonal cathode grids strung continuously from single wires. The current pulse generated in the cathode circuits by the neutron reaction with ³He gas

within the detector reaches the two ends at different times. The difference in rise times of the pulse is used to locate the x-y coordinates of the event. The analog signal produced by the total energy discrimination and risetime circuitry is digitized by a fast analog to digital converter and passed to a fast time-of-flight clock which latches timing information to the position information. The data is passed on to a high speed digital data acquisition system designed through a LASL-ORNL collaboration for use with two-dimensional position-sensitive detectors when a third parameter, such as time-of-flight, must be monitored. This data acquisition system presently includes a half megaword of MOSTEK memory and a unidirectional 24 bit data bus with two control lines. The data can thus be stored in memory very quickly and can be accessed via a standard CAMAC dataway for computer processing. A block diagram of the acquisition and analysis system is shown in Fig. 18. The system is fully described in a joint ORNL/LASL report, ORNL/TM-7325 or LASL-8260-MS by R. Hendricks, P. A. Seeger, J. Scheer, and S. Suehiro.

Data Reduction: The principal software problem involves the processing of the time-of-flight data from megaword sized histograms to simple reciprocal lattice intensities which can be analyzed with existing structural analysis software. A software package has been created for this purpose as a part of a continuing collaborative effort between ANL and LASL staff. It is anticipated that with an instrument of this complexity problems may arise which will require modeling corrections in the data reduction and processing. The reduced data will be analyzed with the LASL Crystal Structure Program Library.

Experimental Data: Preliminary data has been collected on several single crystals of inorganic and organometallic compounds. Histograms collected from a potassium sulfate crystal, covering almost a complete independent unit, are being used primarily for characterization of instrument parameters. Fig. 17a shows a raw data contour plot from one three dimensional K_2SO_4 histogram which has been compacted in the direction perpendicular to the incident beam and is displayed as 2θ vs. time (or wavelength) in four resolution segments. The (011) lattice line is indicated with the dotted line. Figure 17b shows the raw intensity of a single resolution element on the detector face (corresponding to the same (011) lattice line) plotted vs direct wavelength in Å. The signal-to-noise

for the K_2SO_4 data is remarkable and much better than what we saw for hydrogeneous samples.

C. Special Environment Diffractometer SED

A geometrical time focused special environment diffractometer has been in operation for the last two years at the WNR facility. This has been used for powder diffraction by the profile refinement method at high pressures and temperatures. The primary object of study has been the phase diagram of Pu.

Recently, the instrument has been rebuilt to improve the data rate. The new instrument has a source to sample distance of 6 m, a sample to detector distance of about 1 m, and two banks of 12, 1/4", 40 atm 3He detectors geometrically time focused at an angle of 90° . The shutter-collimation system views a 3" x 4" moderator area time focused at 22.5° and produces a beam size at the sample of 3/16" x 1 1/2". The geometry is such that incident and scattered neutron paths cross inside the sample, so that there are no Bragg peaks from the sample vessel. With this new design we anticipate that it will take about one hour to obtain a good powder pattern at current neutron fluxes. The sample vessel in use can currently study pressures up to 5 kbar and temperatures up to $350^\circ C$. The instrument is shown in Fig. 19. Tests with the new instrument are about to begin.

ACKNOWLEDGMENT

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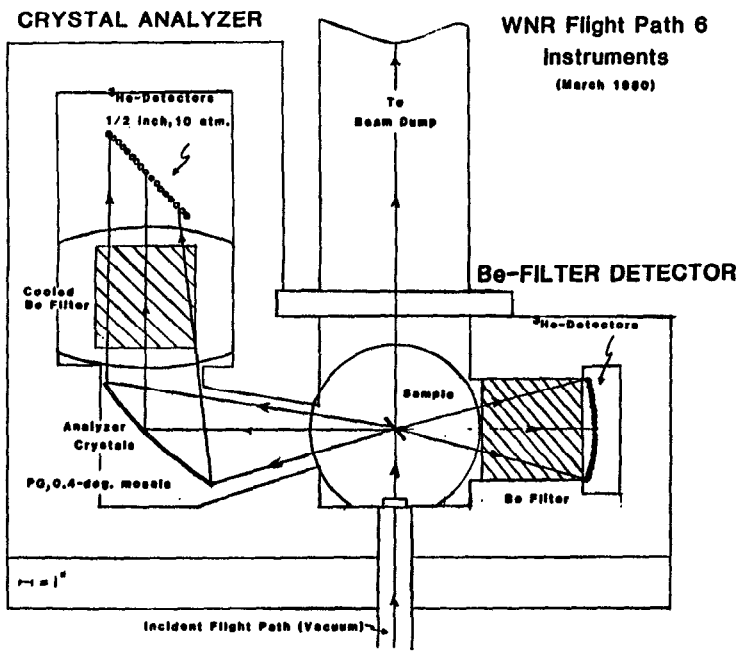


Fig. 2. Inelastic neutron scattering spectrometers at flight path 6 of WNR as of March 1980. Source-to-sample distance is 6.33 m, sample-to-detector distance 1 m for the crystal analyzer, 0.45 m for the Be filter.

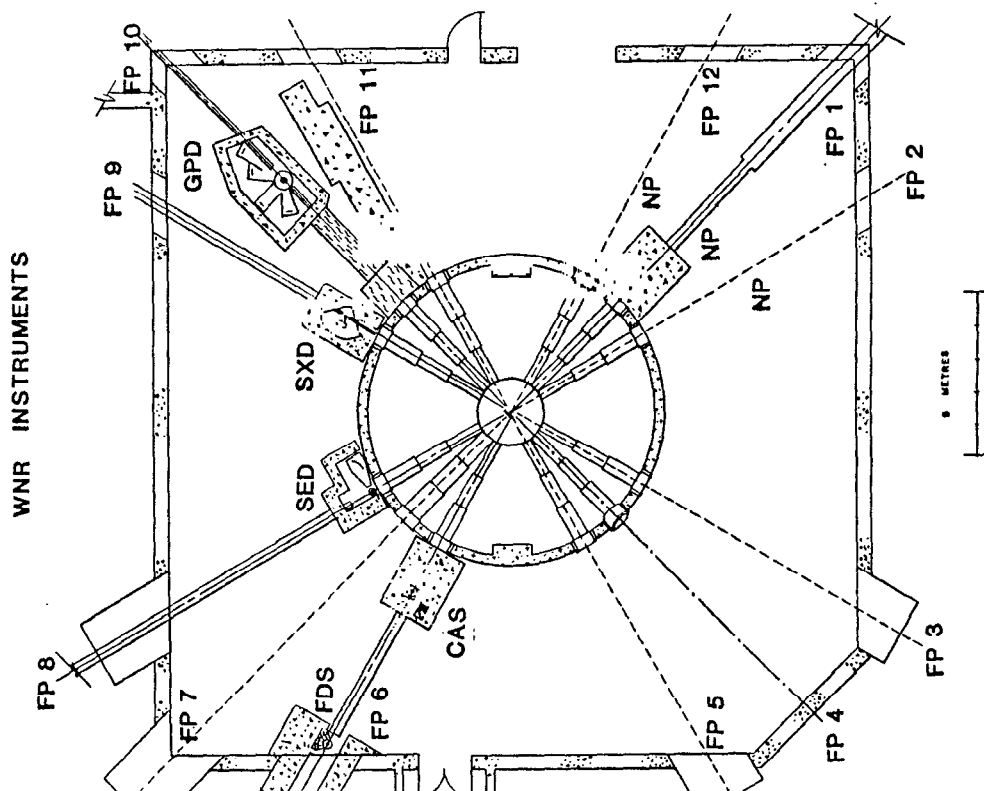


Fig. 1. Schematic layout of instruments in the experimental hall of the WNR.

CRYSTAL ANALYZER SPECTROMETER

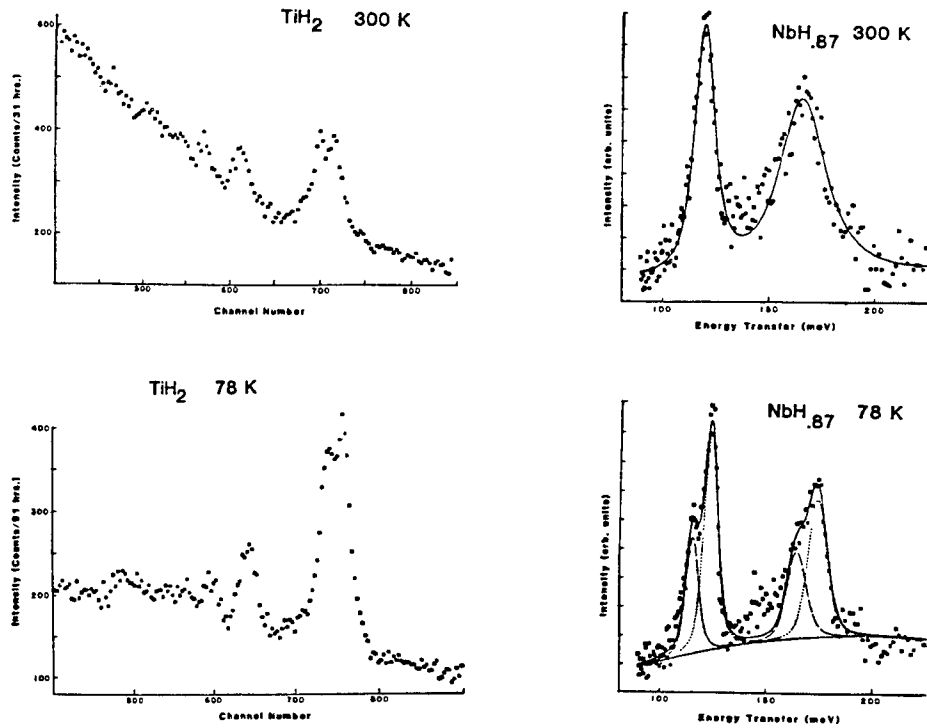


Fig. 3. (Left) Raw inelastic neutron scattering spectra of TiH_2 taken with the crystal analyzer of the radial flight path 5 (top) and the tangential flight path 6 (bottom). The beam area was four times larger at flight path 5. The Be filter was not cooled in either case. Each data point represents an average of three $3.2 \mu\text{s}$ channels.

Fig. 4. (Right) Hydrogen local mode spectra in $\text{NbH}_{.87}$ at two temperatures. The data has been corrected for background and the incident spectrum. Each data set required approximately 24 hrs. of beam time at 120 Hz and $3 \mu\text{A}$.

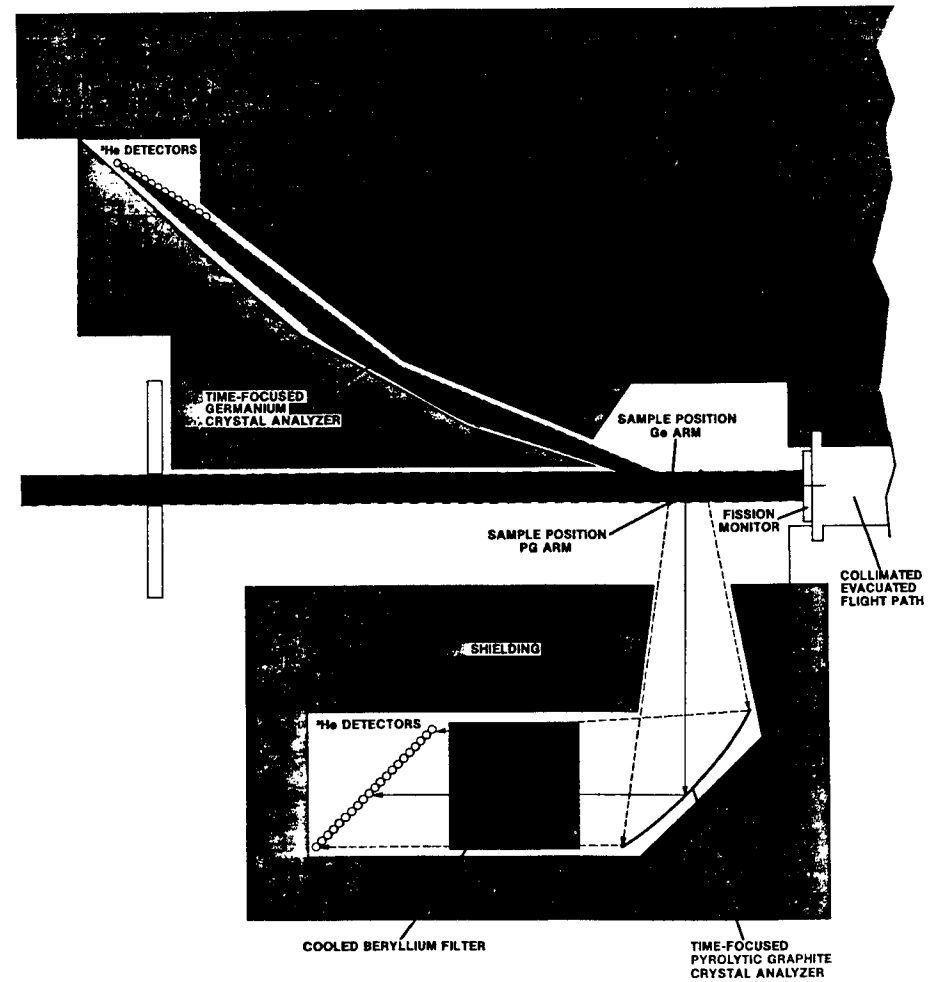


Fig. 5. Crystal analyzer with second, Ge-analyzer ($E_f = 50 \text{ meV}$) planned for early 1981.

BERYLLIUM - BERYLLIUM OXIDE DIFFERENCE SPECTROMETER

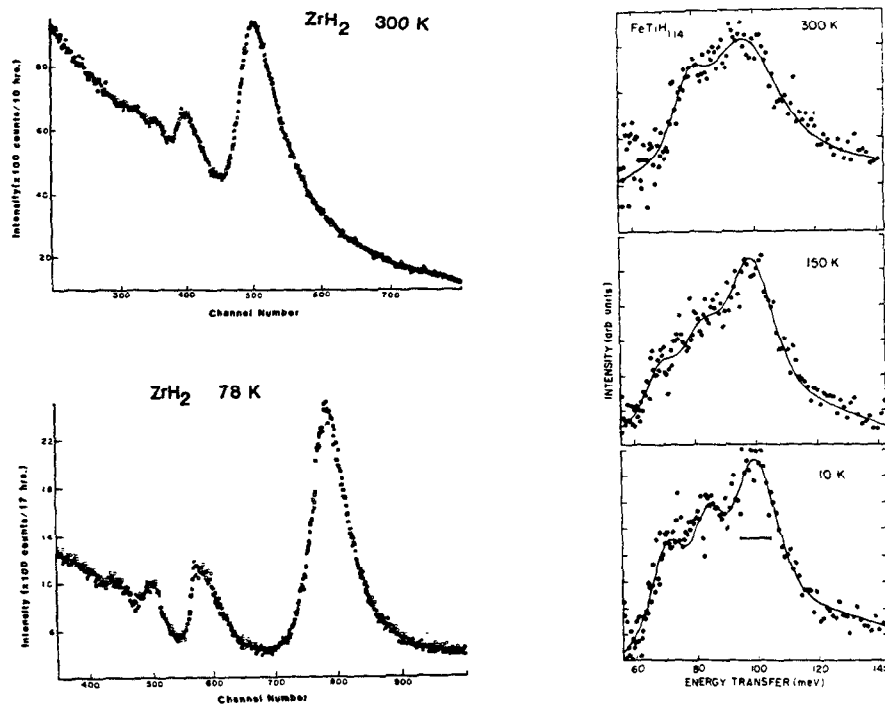


Fig. 6. (Left) Raw inelastic neutron scattering spectra of ZrH_2 taken with the Be filter detector spectrometer at flight path 5 (top) and flight path 6 (bottom). The ratio of final over initial flight path length improved by a factor of four from top to bottom.

Fig. 7. (Right) Corrected inelastic neutron scattering spectra of $FeTiH_{14}$ (β -phase) as a function of temperature obtained on the FDS. The contributions of three filter sections were added after correcting each data set.

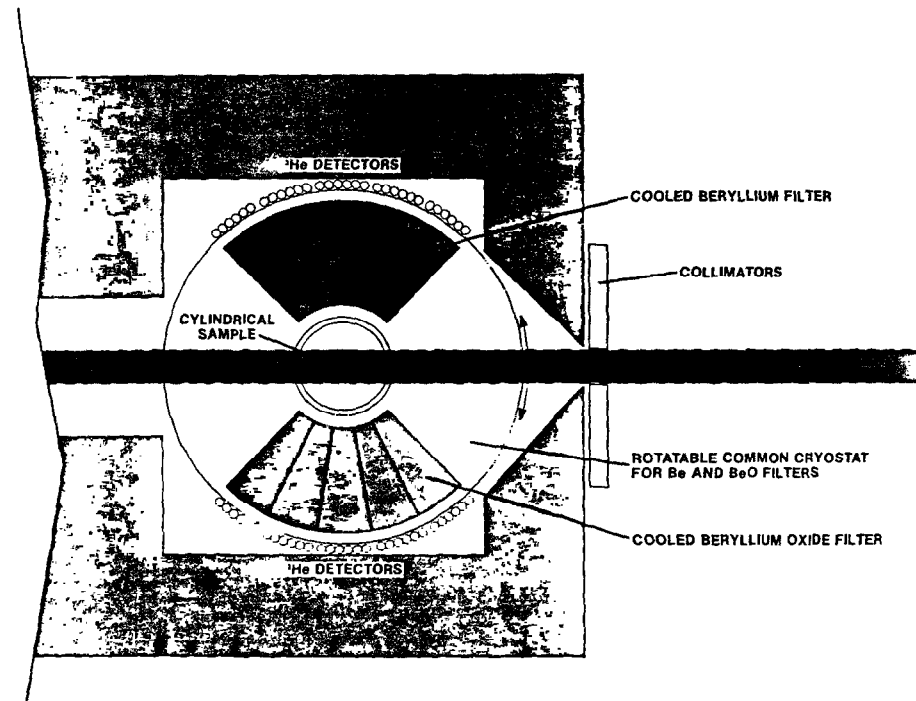


Fig. 8. Be/BeO difference filter instrument presently under construction.

W N R CHOPPER CONTROL

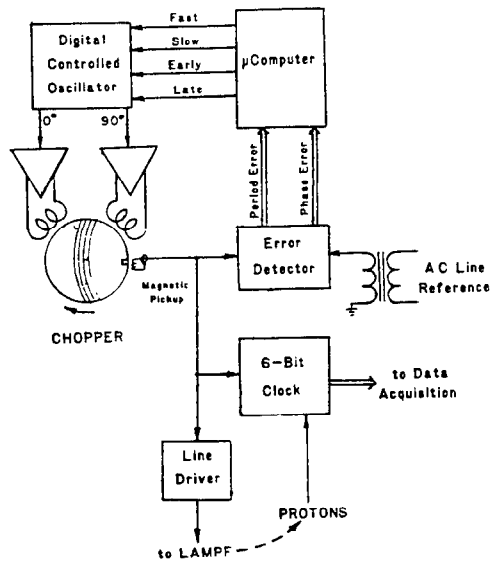


Fig. 9 (Left) Schematic of the chopper control system.

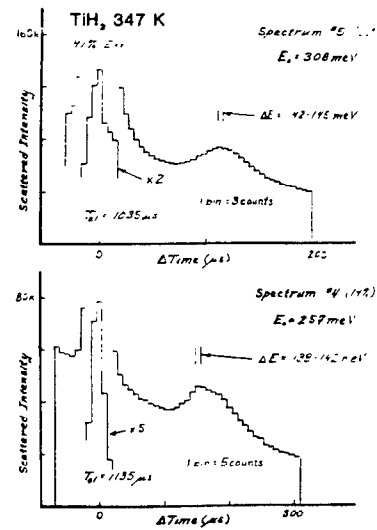
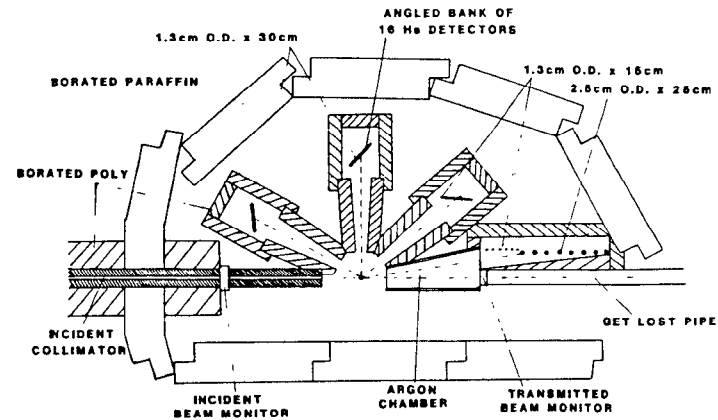
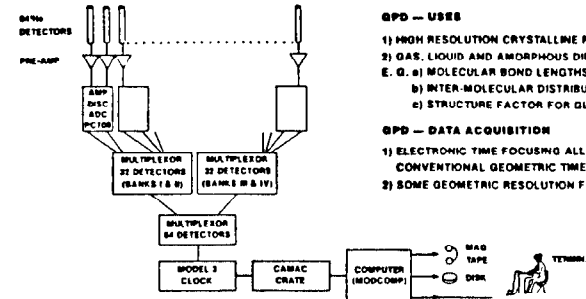


Fig. 10. (Right) TiH_2 spectra obtained with the chopper spectrometer. The overall efficiency for 8 spectra corresponding to eight different incident energies was 91%, with 30% of the scattered neutrons falling into spectrum 5 ($E_0 = 308$ meV).



GENERAL PURPOSE DIFFRACTOMETER (GPD)



GPD - USES

- 1) HIGH RESOLUTION CRYSTALLINE POWDER STUDIES - LARGE AND SMALL D-SPACINGS
- 2) GAS, LIQUID AND AMORPHOUS DIFFRACTION OVER A BROAD Q RANGE.
- E. G. a) MOLECULAR BOND LENGTHS IN FLUIDS
- b) INTER-MOLECULAR DISTRIBUTION FUNCTIONS
- c) STRUCTURE FACTOR FOR GLASSES

GPD - DATA ACQUISITION

- 1) ELECTRONIC TIME FOCUSING ALLOWS LARGER SOLID ANGLE DETECTORS THAN CONVENTIONAL GEOMETRIC TIME FOCUSING, I.E. GREATER COUNT RATES
- 2) SOME GEOMETRIC RESOLUTION FOCUSING WILL SIMPLIFY BINNING OF DETECTORS IN A BANK.

Fig. 11. (Top) Schematic Layout of the General Purpose Diffractometer. The sample is located 10m from the target.

Fig. 12. (Bottom) Data acquisition system for the GPD. The present preamplifier is a LeCroy TRA 510.

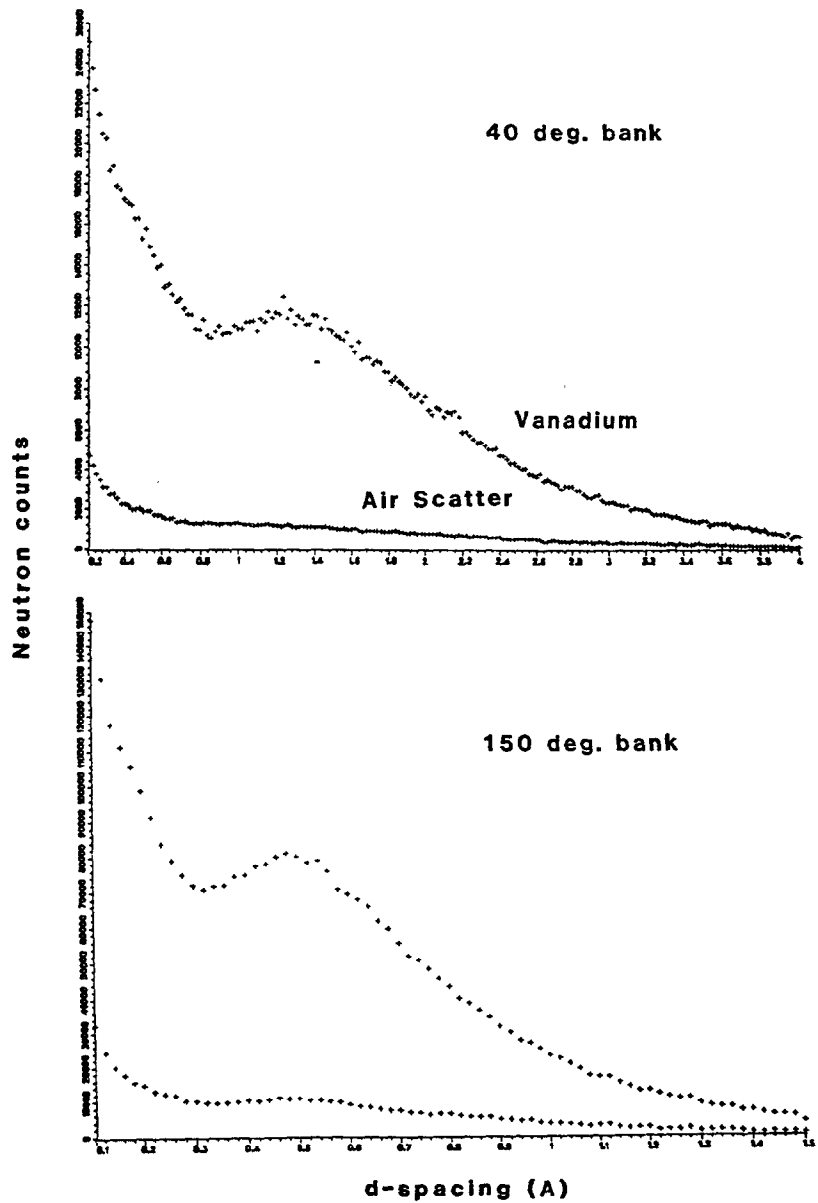
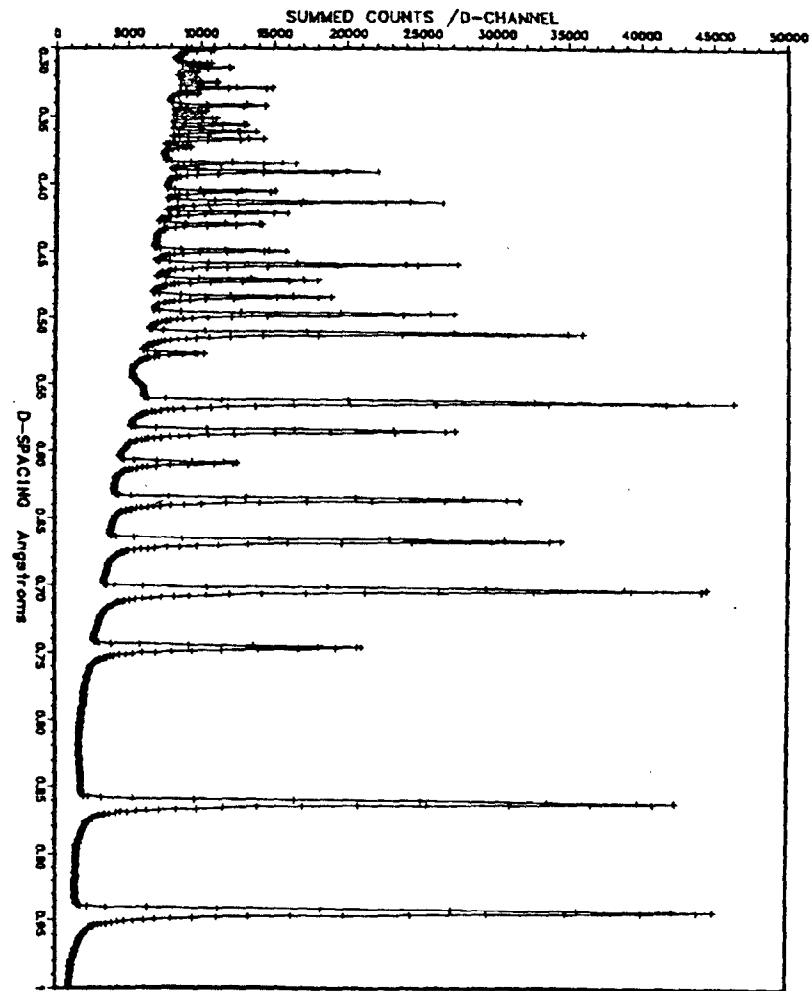


Fig. 13. Raw vanadium and air scattering data for 40° and 150° banks. The detectors are combined in 'd'-spacing bins of width 0.025 Å. These data were obtained in about 12 hrs., running at 2.3 μ A.

Fig. 14. Raw powder pattern from MgO. 15 detectors in the 150° bank have been grouped into the appropriate d-bins by software.



GPD026 MgO 15-150deg 0.0005 d-bins 26.4 μ A-hr

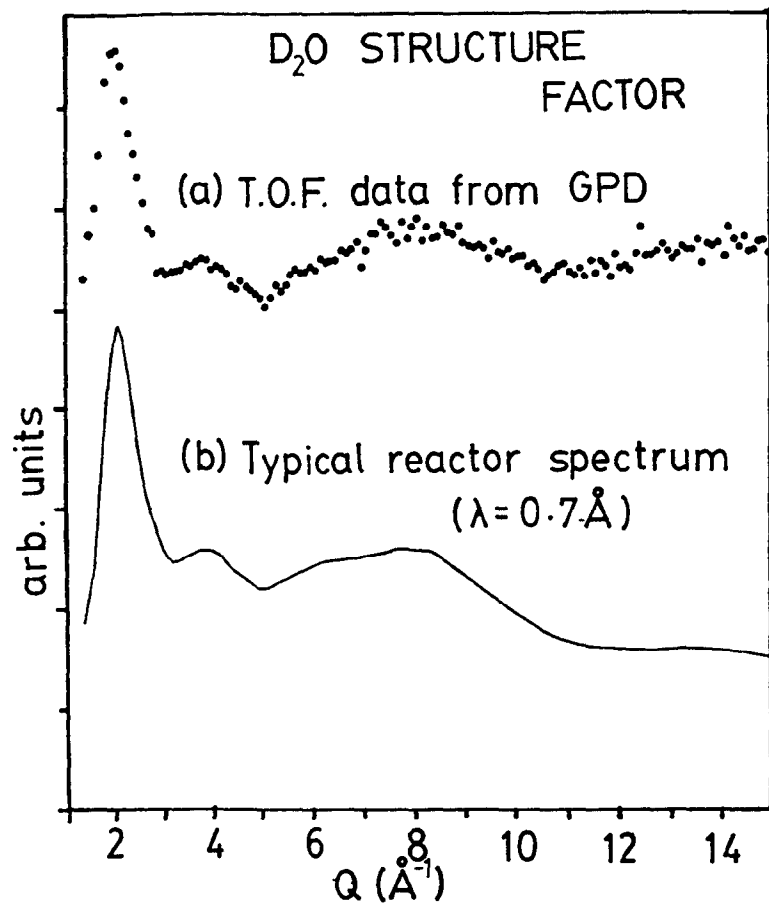


Fig. 15. Neutron time-of-flight spectrum from D_2O at 40° scattering angle. The data were normalized as in Fig. 14. They are compared with a spectrum for D_2O obtained at the I.L.L. All the features at the reactor spectrum are observed, and the Placzek effects are much less noticeable.

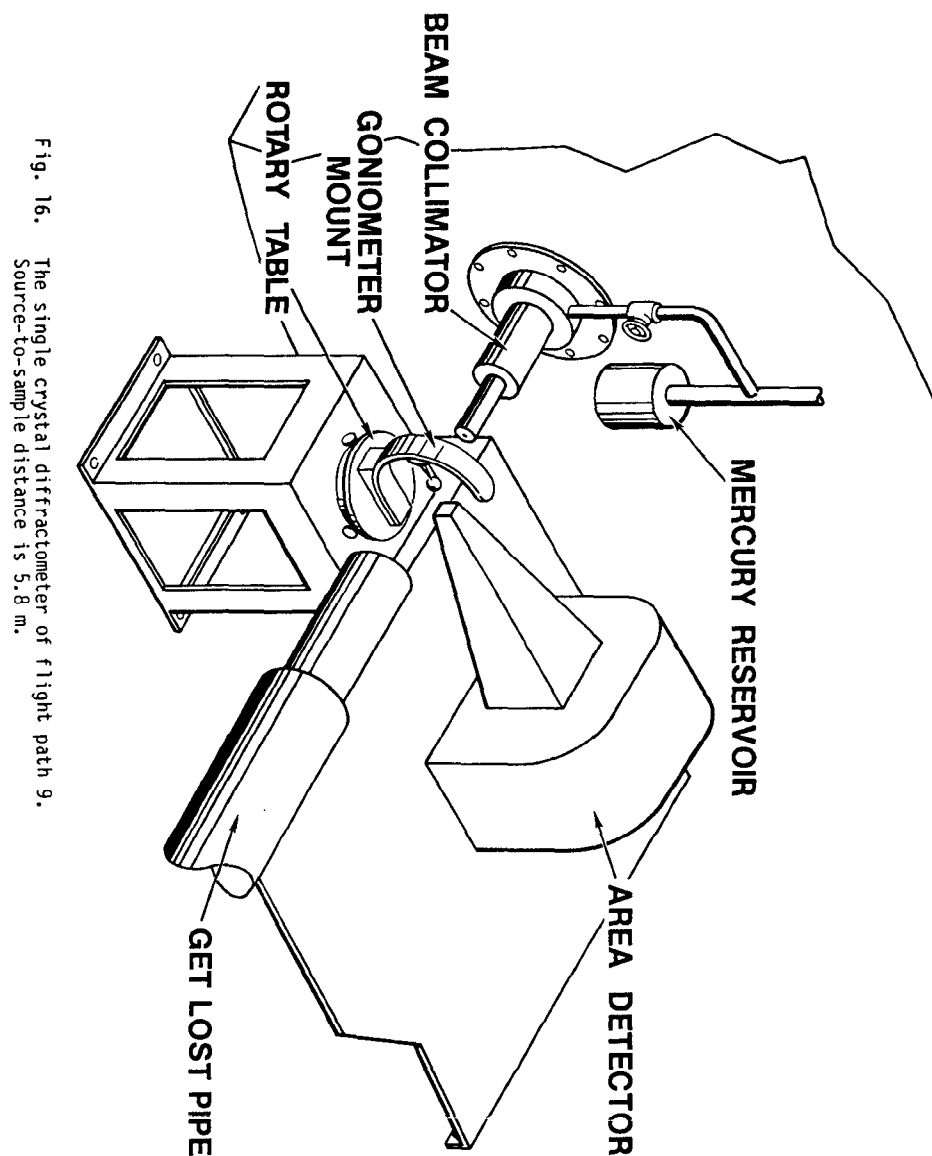
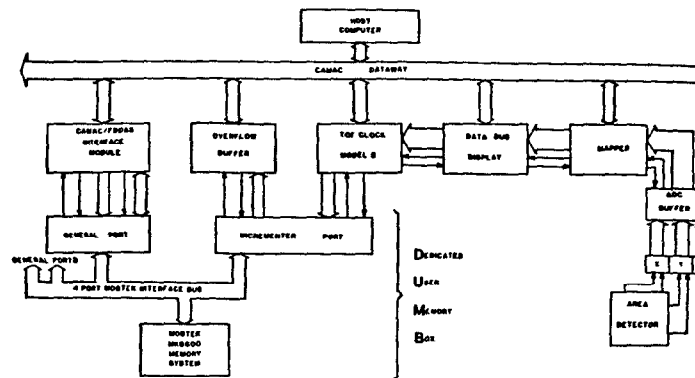
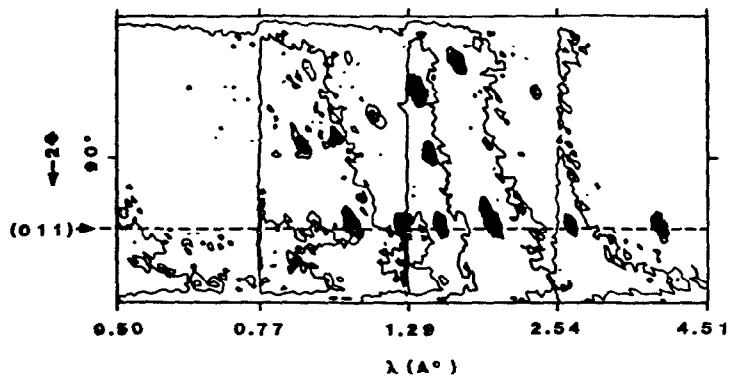


Fig. 16. The single crystal diffractometer of flight path 9. Source-to-sample distance is 5.8 m.



SPECIAL ENVIRONMENT DIFFRACTOMETER

CHARACTERISTICS AND USES

- MIN ~ 0.7 Å
- PRESSURES UP TO 5 kbar AND TEMPERATURES ~ 350°C
- NO SAMPLE VESSEL CONTRIBUTION TO POWDER PATTERN
- PROFILE REFINEMENT CODE CAPABLE OF UP TO THREE COEXISTING PHASES
- AT SHORT 7m FLIGHT PATH AND 120Hz, FLAME OVERLAP IS INSIGNIFICANT
- USES: FOR STRUCTURAL STUDIES OF POWDER SAMPLES AT HIGH PRESSURES AND A WIDE TEMPERATURE RANGE.

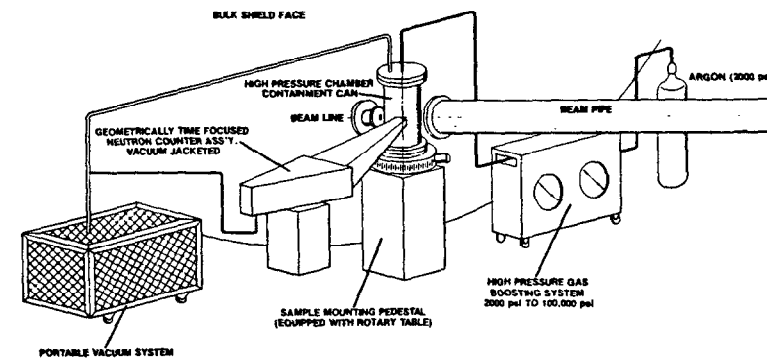
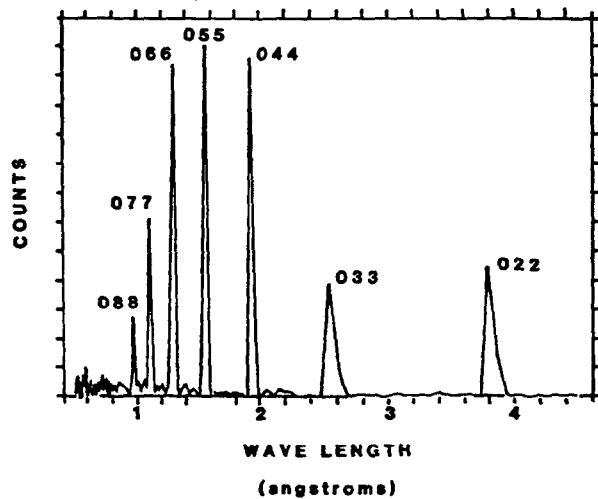


Fig. 17a (Top) Contour plot of a typical K_2SO_4 histogram containing the (011) lattice line.

Fig. 17b (Bottom) Intensity vs wavelength for one resolution element containing the (011) line.

Fig. 18 (Top) Block diagram of the data acquisition system for the position-sensitive detector at the single crystal diffractometer.

Fig. 19 (Bottom) View of the special environment diffractometer at flight path 8.