NEUTRON BEAM RESEARCH

at Rutherford Appleton Laboratory

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Neutron Beam Research

The dominant project in this part of the Laboratory programme is the construction of the Spallation Neutron Source (SNS) and its neutron scattering instruments. Laboratory staff also carry out neutron scattering research and development, often in collaboration with university scientists, and technical support is provided for university neutron beam research programmes, mostly at the Institut Laue-Langevin, Grenoble but also at AERE, Harwell.

The Spallation Neutron Source

Following the initial achievement in January, beams of 70 MeV H^- ions have been run on a number of occasions through the transfer line to the point of injection into the synchrotron. During November, 70 MeV H^- ions were steered into the straight section of the synchrotron. The complex equipment for converting the H^- ions into protons and projecting them into the right direction for acceptance by the synchrotron was successfully used to produce protons as required.

All the components to reach the next milestone are available (Fig 4.1). Its achievement has been held up by the delivery of the main dipole magnets for the synchrotron, but the last of these was delivered early in December and the synchrotron ring completed on 16 December. The aim is to use a synchrotron ring with a complete vacuum system and two of the 6 eventual radiofrequency accelerating cavities to enable protons to be injected, collected by the magnet system and trapped by the radiofrequency system. The vacuum system is expected to be complete and run during December. Work is proceeding on equipment to accelerate the protons to 550 MeV using a total of 4 RF cavities and then to extract them into a beam dump in the synchrotron room. Good progress is also being made on the target station where a major component, the 3 m diameter stainless steel vessel which will contain the target and moderator system, was installed in December. By October 1984 it is expected that work will be complete for production of first neutrons. This requires completion of the extracted proton beam and the target station. It is expected that it will take two years to run up from the initial low (approximately 10%) intensity to full performance of 200 μA of 800 MeV protons.

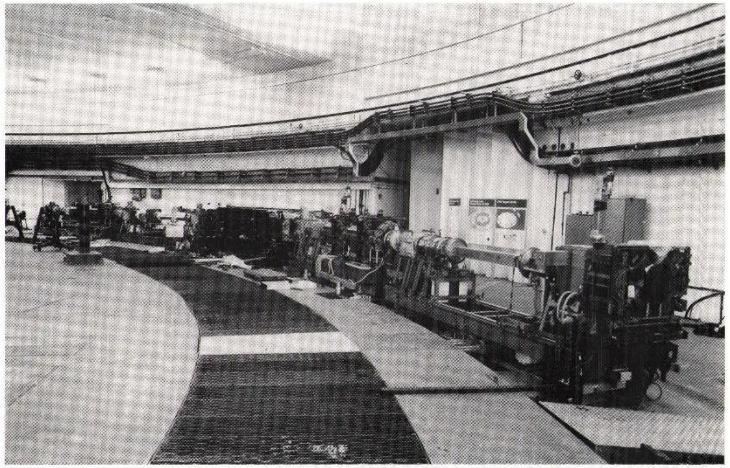


Fig 4.1 Part of the synchrotron showing a dipole magnet joining two straight sections. (Photo 83 RC 4236)

The 70 MeV Injector

The injector system consists of an H^- ion source, a 665 kV dc accelerating column, four Alvarez accelerating cavities taking the energy to 70 MeV and a transfer line to take the H^- ions to the synchrotron. The system has been run regularly throughout the year. These runs have been of short duration to enable the synchrotron installation to continue and to conserve available manpower. The running time has been used to improve the reliability of the equipment, to do beam dynamics studies aimed at producing the required quality of beam for the synchrotron and to minimise beam losses which at full power could produce induced activity in the components. To minimise radio-activity problems during commissioning work, the mean current is kept below 1 μA compared with the design intensity of 400 μA. This is achieved by reducing the repetition rate from the design value of 50 Hz to about 1 Hz and by shortening the pulse length from the design value of 500 μs to less than 100 μs. Typical currents during the pulse are 5 to 7 mA compared with the design level of 20 mA. Under these conditions the emittance (quality) of the beam is as expected. Typical values are 12.5 π μrad m horizontally and 25 π μrad m vertically. The beam loss along the linac, when scaled to full power, is at an acceptable level. The linac and transfer line are well equipped with diagnostic equipment to enable beam current, position and profile to be measured. This equipment has been successfully controlled, as has an increasing number of components, by the injector computer control system.

A number of sources have operated satisfactorily but they still require some improvement. The ion source, as with any complex equipment, would be expected to work more reliably during long uninterrupted runs. The RF system for the linac tanks requires further work to enable control through the computer system and to provide more automatic control of tank voltage and phase levels. The stability of the power supplies for the linac and the transfer line magnets has been improved to a satisfactory level for routine operations. Initial commissioning has been done using the beam loss monitors which during routine operation will give the operators information on beam losses to enable induced activity levels to be minimised.

The 800 MeV Synchrotron

Injection

The components of the injection system are a steering magnet, to sweep the beam vertically during the 500 μs pulse of H^- ions, followed by a septum magnet which directs the ions into the straight section of the synchrotron. Here, the H^- ions are stripped of their 2 electrons by a transparent 0.25 μm foil of aluminium oxide. Four pulsed magnets control the orbit of the incoming H^- ions and the protons subsequent to the stripping process so that the protons from the foil follow the orbit of protons which have already been injected. This system, shown diagrammatically in Fig 4.2, is designed to achieve in the most economical way the build up of the required high proton current in the synchrotron. Initial trials were carried out in November with beam through the system. H^- ions were successfully stripped by the foil, and protons detected by scintillators and a toroid beam current monitor in the straight section. The 14,000 A pulse magnet power supply has been commissioned to work at full power.

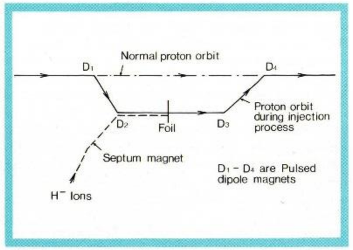


Fig 4.2 Schematic of injection process. (83 MB 6051)

Synchrotron Ring Magnets

The magnet system was completed in December after delivery of the last of the ten dipole bending magnets. On arrival, they were compared magnetically with the first production dipole used as a standard, and found to be acceptable. At injection levels the mean field integral is within 0.01% of the design target, with an rms deviation of 1.2 parts in 10^4 rising to only 1.7 parts at extraction, even though some of the mechanical tolerances were not met in full. If necessary, fine corrections can be effected by adjusting the magnets' radial positions in the ring. All the magnets were surveyed into position for initial injection studies.

Synchrotron Magnet Power Supplies

The power supply for the main magnet system was connected to the magnets and commissioning of the overall system commenced. Individual components of this system such as the dc motor-alternator which makes up energy lost in the magnet system were commissioned during the year.

Synchrotron Vacuum

The vacuum system for the complete ring was connected up during December. Earlier in the year about half of a straight section was tested successfully and it was decided that the ring would not be vacuum tested in sections since this would have required extra supports on some components to carry the additional vacuum load.

RF Acceleration System

The two cavities required for trapping studies were installed in the synchrotron and tested to full power. The final commissioning took place during November and December. This involved the accurate control of the phase relationship between the two cavities with the frequency being swept between 1.3 and 3.1 MHz during a 10 ms half sine wave period. This required the commissioning of the complex low-level analogue and digital electronics and the high current regulators for the cavity ferrite bias which changes the tuned frequency of the cavity. Trapping studies will use class B amplifier systems. Later operation at high intensity in the synchrotron will require the parallel class A system which will compensate for the beam-induced voltage in the cavities. The overall system has been designed to take the class A system which was further developed during the year. For full operation, 6 RF systems will be required. The power supplies for all 6 systems, and bias regulators for 4, were installed and work on the remaining cavities and amplifiers continued. A large amount of cabling and termination work has been done for the RF system.

Synchrotron Diagnostics

The beam dynamics of the protons in the synchrotron need to be well understood to ensure operation to the full design intensity and to minimise beam losses and hence induced activity of components. A large range of diagnostic equipment was installed in the synchrotron during the year. This included two beam intensity monitors, a total of 33 monitors for measuring vertical and horizontal positions of the proton beam within the vacuum vessel, five profile monitors which measure the density of protons across the aperture of the vessel and the system for measuirng the betatron frequency of the protons. In addition, the diagnostic equipment for commissioning the injection system was installed and successfully used. As with the RF system, a large number of cables were installed and terminated.

Beam Loss Protection

During the year, the collector system was manufactured ready for installation. Beam loss monitors were installed along the length of the linac and the injector transfer line, and were successfully commissioned. Similar devices will be installed around the synchrotron and provisioning continued during the year.

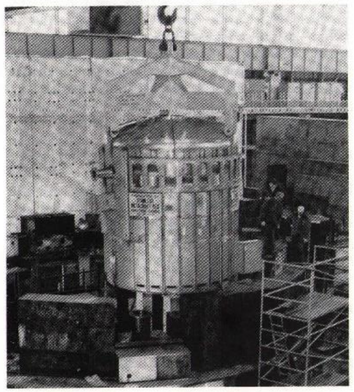
RF Shields

For the synchrotron to operate at high intensities, the proton beam must have surroundings with a low RF impedance, otherwise voltages would be induced which would feed back on to the beam and blow it up so that it could not be contained within the vacuum chamber. The SNS synchrotron has specially designed RF shields to provide this low impedance. During the year, these shields (an accurate array of wires and plates) were successfully fitted to all ceramic chambers and bellows units in the vacuum system. Of special note was their fitting to the curved ceramic chambers (4.8 m long with 7 m radius of curvature) in the dipoles. The inside dimensions of the chambers, which are not machined, were measured using an accurate curved beam, with position sensors fed to a punched paper tape. This allowed machining of the spacers supporting the shield, to ensure that the shield was accurately positioned with respect to the expected proton beam orbit. RF finger strips at the ends of the chambers support the shield assembly to allow for expansion and contraction in the event of a temperature change. The assembly procedure was successfully proved to allow installation in the synchrotron.

Extraction System

This will be required for extraction studies by mid 1984. The main components are three ferrite-cored kicker magnets which deflect the 800 MeV protons into the mouth of a septum magnet which gives a further vertical deflection of protons out of the synchrotron. The kicker magnets work at 37 kV and 5300 A with a rise time of about 200 ns. Two deuterium thyratrons are switched to discharge a lumped delay line into each magnet. Installation and testing work has continued throughout the year. One prototype magnet has been successfully pulsed to the required specification from two installed thyratron units. All components have been delivered or ordered.

Fig 4.3 The target void vessel. (83 RC 5760)



The Extracted Proton Beam Line (EPB)

This transports the extracted protons over the synchrotron, down to within 1.9 m of floor level and along a shielded tunnel to the target station. The special bending magnet which deflects the beam back to the horizontal after its extraction was installed on its stand and plinth. Stands to support other EPB magnets in the synchrotron room were delivered. Magnets already available were refurbished during the year and the line surveyed for installation. Concreting of the side walls of the shielding tunnel was completed together with the grouting of the steel shielding which consists of blocks and Nimrod magnet sectors.

The Target Station

Inside the target station is a depleted uranium target in which each 800 MeV proton produces about 25 neutrons with energies of about 1 MeV. The neutrons are slowed down in moderators of hydrogenous material to energies in the meV to eV range. Neutrons which would be lost are deflected back into the moderators by a reflector system. The target/moderator/reflector assembly is contained within a large (~ 3 m diameter) stainless steel void vessel. This is surrounded by biological shielding which is ~ 4.5 m thick. Neutrons leaving the faces of the moderators are channelled through 18 holes in the shielding to the spectrometers used by experimentalists. The programme date for first neutrons is October 1984.

Target Assembly

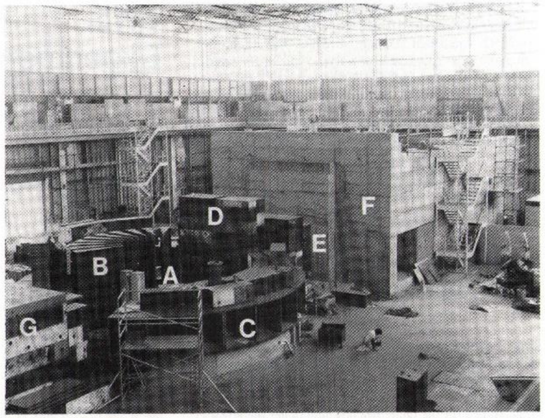
The successful development of zircaloy cladding of uranium plates was completed during the year. Sets of plates were ordered for two targets. The plates will be held in vessels and cooled by manifolds which were also ordered as were the reflector vessels, which hold beryllium cooled by heavy water, and various decouplers. Orders were also placed for the hydrogen and methane refrigeration systems for the two cold moderators, the hydrogen moderator being at 25 K and the methane at 95 K. A test cold moderator vessel designed to achieve maximum strength for minimum thickness was subjected to stringent tests and since the results confirmed the design, orders were placed for the vessels. There were problems in the manufacture of the stainless steel target void vessel but it was delivered in November having passed the stringent safety tests required of a reactor-type vacuum vessel. It was installed in position in the target station (Fig 4.3).

Bulk Shield

Some target station components are shown in Fig 4.4. Each of the 18 neutron ports can be closed off by shutters of steel ~ 2 m thick. These shutters will be held in position by shielding wedges of steel. All the wedges were delivered during the year and a trial installation carried out to achieve the vertical alignment required of ~ 1 mm. A trial fitting of a complete shutter was also successfully carried out. The wedges were removed to allow the fitting of the void vessel. The shutters were also delivered together with their operating mechanisms.

Fig 4.4 Target station components. (83 RC 4243)

A Target position. B Wedges for supporting shutters. C 'Inserts' to allow hand-stacking to make neutron holes. D Part of main shield. E Remote handling cell position. F Services area shielding. G Extracted proton beam tunnel.



Work has continued on the installation of the massive steel and concrete biological shield. A trial installation of shielding was completed within the inserts which allow tailoring of the neutron port to meet the experimental requirements. The bridge which supports the shielding over the void vessel was delivered in November and has been installed.

Remote Handling and Services Areas

After use, the target/moderator/reflector assembly is withdrawn on rails into the remote handling cell for disassembly and replacement. The same rail system extends into the shielded services area. Trolleys on the rail system hold the steel shielding door (which closes up the back of the void vessel), the services which cool the target and the refrigerator systems for the moderators.

A drainage system to cope with any unlikely spillage of radioactive liquids was completed during the year and the rail system installed, aligned and grouted in. The civil engineering for the remote handling cell was almost completed and the services area built. The remote handling cell work allowed for the lead bromide shielding windows (for viewing the assembly in the cell) and tubes to take the two pairs of remote manipulators. Ventilation systems for the target station areas were designed, ordered and some components installed. Services systems for the target station were designed and many ordered.

Control System

Work continued on the control system based on a hierarchy of a minicomputer, a microcomputer and a hardware system. The electronic systems are being built and tested and programs written for operating various parts of the target station. The target station control room has been built and a start made on the installation of its contents.

SNS Control System

This is based on four minicomputers. The injector computer has been used throughout the year and the number of components controlled through it increased. It has been used to control the diagnostic equipment, to collect data, and to analyse and display the results. This has provided very useful experience for the remainder of the control system. Some changes have been made to the system software to improve response times. The synchrotron computer was installed and used to develop the synchrotron diagnostic equipment. During November the synchrotron computer was connected directly to the main control console for the first experiment of beam into the injection straight. In December, for the second experiment, the console computer was used, coupled to the synchrotron computer via the message transfer system. Interface hardware was provided as individual components and systems of the synchrotron were installed. The fourth computer, that destined for the target station, was used for development work.

Safety Assessment

A safety assessment of the SNS was completed which showed that the SNS will be safe to operate within the legal requirements. A major conclusion is that with the proton beam turned off the target will not melt under the effect of radioactive heating. A major design feature of the target station control system is to ensure that the proton beam is cut off when there is any target station malfunction.

New safety regulations expected to come into force in 1985 will require a hazard survey of facilities like the SNS. The new regulations have been anticipated, the survey completed and a preliminary version sent to the Health & Safety Executive Inspector; his comments were favourable. It is also necessary for the Department of the Environment to be notified about the normal releases, albeit small, of radioactive material to the environment. Following a preliminary report, the indication was that the Laboratory's Certificate will be updated to take account of the SNS.

Future Developments

As part of the collaboration with KFA Julich, West Germany, improvements to the SNS existing target arrangement together with a possible second target station optimised for longer wavelength neutrons have been investigated. Julich has also proposed collaborative experiments at the SNS aimed at validating results from theoretical studies using complex computing programs. Six Julich staff have been working on the SNS machine and target station for seven months during the year.

SNS Experimental Facilities

The First Six SNS Instruments

The ultimate capacity of the SNS target station for neutron scattering instruments is in the region of 20 to 25. As a first step, seven instruments were identified and approval given for their construction. These were chosen to give a balance between the different criteria for exploiting the novel features of the SNS, doing new science as soon as possible, and satisfying existing user demand. As a result of financial restrictions only six of these instruments will be operational by the time the first neutrons are produced. The seventh, the *High Intensity Powder Diffractometer*, will be built when funds are available. All of these decisions were taken in consultation with the user community via the medium of the SNS Science Planning Group whose role is to advise the Laboratory on the scientific exploitation of the SNS.

Two instruments have already been built and are operating on the Harwell Electron Linac HELIOS. The first of these is the *Liquid and Amorphous Materials Diffractometer* designed to study the structure of non-crystalline materials with high intensity up to high scattering vectors and also to serve as a medium resolution powder diffractometer. The second is the *High Throughput Inelastic Spectrometer* which was envisaged as a very high intensity but moderate resolution vibrational spectrometer. An improved version of this spectrometer is now at the design stage. Two further instruments are each unique neutron scattering spectrometers. The *High Resolution Powder Diffractometer* will have the best resolution ($\Delta d/d \sim 4 \times 10^{-4}$) of any such instrument in the world and will considerably enhance the utility of the technique of neutron powder diffraction. The *High Energy Transfer Spectrometer* will enable higher energy transfers to be measured with better resolution and at lower momentum transfers than has so far been possible. This will permit new types of investigations to be made on vibrational and magnetic excitations. The remaining two instruments will serve current growth areas, where user demand is very high, and they will also provide novel features not available on the corresponding reactor instruments. The *Low Q Diffractometer* will serve the rapidly growing community from all scientific disciplines interested in using the particular features of neutrons to investigate structures on the scale 10 Å to 500 Å. The *High Resolution Inelastic Spectrometer* will enable quasi-elastic and inelastic scattering measurements to be made with energy resolutions in the microvolt region.

The *Liquid and Amorphous Diffractometer (LAD)* is a total scattering spectrometer designed specially for the determination of the static structure factor of liquids and amorphous materials. It has continued to operate routinely on the Harwell Linac. Experiments carried out by visiting university scientists under the SERC/AERE Joint Programme include powder diffraction, and liquid and amorphous structure measurements. During the year, the second batch of detectors was installed to complete the complement of detectors. Calibration experiments have shown that the resolution is as expected, but the neutron intensity is less, due mainly to a lower than expected flux from the moderator. Encouraging features have been the good performance at low angles (5° and 10°) and at high incident energies (⩾ 1 eV). For many of the experiments, the prototype sample changer has been used and has proved reliable. Software for the routine analysis of the data has been written. Raw data can be brought to the SNS HUB Computer (VAX 11/750) for treatment. A full set of programs for calculating the structure factor S(Q) is available together with programs for instrument calibration. These programs will serve as a basis for the SNS versions.

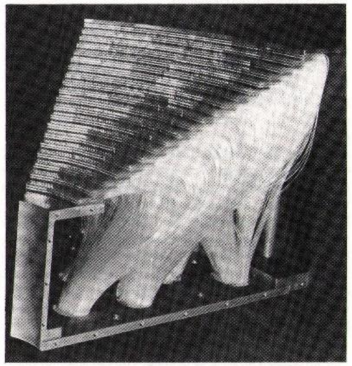
The next generation instrument in this field is the *Small Angle Neutron Diffractometer for Amorphous and Liquids Studies (SANDALS)*. Its design has been reviewed in the light of experience gained on both reactor and pulsed source instruments. These results have shown that one of the major corrections, the inelasticity or Placzek correction, decreases with decreasing angle and increasing incident energy. The new design will concentrate on lower scattering angles (0.5° to 50°) and will use thicker scintillator detectors to increase the detection efficiency at higher neutron energies. These changes will allow a complete determination of the structure factor from relatively low scattering angles.

The *High Throughput Inelastic Scattering Spectrometer (HTIS)* is an inverse geometry spectrometer intended to complement the traditional infra-red and Raman scattering techniques in chemistry, physics and material science. It has a cooled beryllium energy analyser which, due to its large solid angle, provides high data rates for the vibrational spectroscopy of incoherent scatterers. It has been successfully installed on the Harwell Linac, and is now a scheduled user instrument. A number of well characterised molecular and metal hydride systems have been measured, confirming the predicted instrument performance. Some initial experience has been gained with university users investigating absorbed species and metal hydride systems. Data reduction software, which will serve as a basis for the SNS software, has been implemented and several alternative methods of data analysis have been investigated.

A number of different energy analysers have been considered for incorporation on HTIS to improve energy resolution and lineshape. This work has culminated in the design of a *Time Focused Crystal Analyser Spectrometer* (TFXA) which will provide greatly improved energy resolution and lineshape at the expense of a modest reduction in count rate. The analyser is a crystal of pyrolytic graphite in a time focused geometry. The sample and detector array are in the same plane and the analysing crystal is set parallel to this plane. All detected neutrons have, to first order, the same flight time through this system. TFXA is currently under construction and will be available with a detector covering half of the eventual solid angle during the early operating period of the SNS. Both analyser systems are designed to be easily interchangeable at the same 12 m flight path. On the Linac, HTIS was modified for a test of a prototype TFXA. The expected improvement in lineshape was observed, and the intensities and resolutions were consistent with calculations.

The *High Resolution Powder Diffractometer (HRPD)* will provide a significantly higher resolution than any comparable neutron instrument. A resolution of $\Delta d/d = 4 \times 10^{-4}$ will be achieved using a total neutron flight path of 98 m which will allow up to 300 structural parameters to be determined. Three major components of this instrument have been completed this year. The first module of the eight module detector has been constructed and tested (Fig 4.5), the diffractometer tank has been assembled and installed (Fig 4.6) and the instrument building has been completed. All of the 1 m neutron guide sections required for the 96 m neutron flight path have been delivered. The testing of the optical quality of these sections, using auto-collimation, has commenced and a contract for the installation and alignment of the guide has been placed.

Fig 4.5 A single octant of the High Resolution Powder Diffractometer's detector. (83 FC 1819)



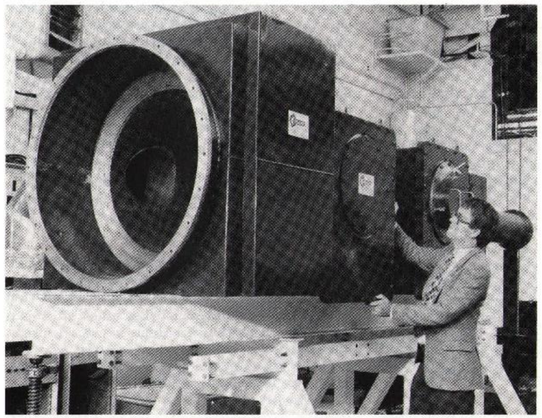


Fig 4.6 The Sample/Detector vacuum chamber of the High Resolution Powder Diffractometer. (83 FC 4399)

A number of computer programs associated with neutron powder diffraction have been implemented on the VAX 11/750. In particular, the Cambridge Crystallographic Subroutine Library (CCSL) profile refinement program has been successfully tested using several different constant-wavelength diffraction profiles. CCSL will serve as the basis for a time-of-flight (TOF) profile-refinement suite of programs at RAL. CCSL subroutines have also been used to create a number of programs associated with both constant wavelength and TOF neutron powder diffraction, including profile simulation programs (see Fig 4.7), peak refinement programs with a number of different peak shape options, peak search routines, and background subtraction programs using orthogonal polynominals.

The *High Energy Transfer Spectrometer (HET)* is intended to cover excitations in the range between 100 meV and 500 meV at well defined values of momentum transfer. Its uses will include $S(Q, \omega)$ measurements on liquids and gases, high energy magnetic excitations and molecular spectroscopy. Detailed design of the instrument has continued and the main components are now being manufactured. The main components of the beamline, the collimation, choppers, vacuum flight paths and shielding should be available for start up of the SNS, together with a full low angle counter bank (3° to 7°), one variable angle high angle counter bank (70° to 140°) and one octant of the 8° to 30° bank. The environment for single samples will be variable from ambient temperature to 20 K and it is hoped to have a multiposition sample changer working to cryogenic temperatures. Development will continue, drawing on early operational experience, and by the time SNS reaches its full intensity it is expected to have a full complement of counters at all angles including a high resolution horizontal bank for single-crystal measurements.

The *Low Q Diffractometer (LOW Q)*: Small Angle Neutron Scattering is a technique used to study a wide variety of phenomena in condensed-matter science concerned with small particle or other inhomogeneity effects on a scale of 10 Å to 500 Å. An early specification for an instrument, called *LOW Q*, which is to be installed on the SNS, has been reviewed critically to incorporate new ideas and experience gained from several years of operation of pulsed source instrumentation at Harwell, KENS and Argonne. A review of fast neutron backgrounds produced by SNS has suggested that an alternative be sought to the originally requested fast neutron chopper.

In view of the success of neutron guides for cold-source instrumentation, a device for bending the instrument off axis, away from the fast beam, has been designed with a super-mirror surface. This is a static device which, once lined up, will demand only minimal servicing. As a result of the bend in the thermal neutron beam ($\lambda \geq 1$ Å) the straight-through fast neutrons can be attenuated before reaching the sample area giving a substantial improvement in signal-to-background. The super-mirror increases the instrument's total length and a new chopper system has been designed accordingly. A set of three double disk choppers of similar external design and drive has been proposed. The design of the detector has been revised. At present, engineering design and development are under way for all major components and it is expected to have a limited form of the instrument in operation when the first neutrons are available from SNS. The components essential to initial operation of LOW Q will be installed by this time but those elements of the design intended to refine LOW Q's performance will be added later, including the high resolution and the fine collimation options. The sample detector flight path will be limited initially to a maximum of 10 m and only two of the nine sectors on the main detector and one of the annular rings will be available. There will be a limited data-acquisition system appropriate to this initial configuration.

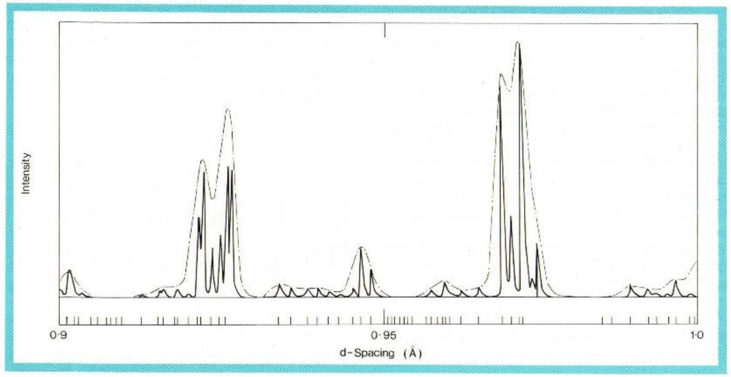


Fig 4.7 The simulated neutron powder diffraction profile of the orthorhombic perovskite $SrZrO_3$ on D1A, ILL Grenoble for $88^\circ \leq 2\theta \leq 101^\circ$: λ = 1.387Å (broken line) and on the High Resolution Powder Diffractometer (unbroken line) showing the effect of the improved resolution. (83 MB 6052)

The *High Resolution Inelastic Spectrometer (IRIS)*: Work has continued on the design of this instrument, which is optimised for the study of near-elastic scattering processes with energy resolutions from 1 μeV to 50 μeV. It will be used to investigate transport phenomena and low-lying excitations in solids. Initially IRIS will incorporate an analyser system which is being built at the Bhabha Atomic Research Centre (BARC) in Bombay as part of a collaborative agreement on the use of the SNS by Indian scientists. This analyser utilises the sharp transmission edges of poly-crystalline beryllium at different temperatures to define the analysed neutron energy and will provide resolution in the range 30 μeV to 50 μeV. The analyser will be delivered in March 1984 after assembly and testing; the cryostats, detectors and beryllium filters have already been tested. RAL will be responsible for the incident beam line and beam definition. The 35 m long nickel-plated glass guide has been ordered and the design of the overlap chopper is completed. The extension to the experimental hall to house both IRIS and LOW Q has begun and completion is expected by March 1984.

Computing

PUNCH (the Pulsed Neutron Computer Hierarchy) is the system of computers and electronics which controls the neutron scattering instrumentation on the SNS. During the year examples of all the major components of the PUNCH computer system have been delivered including the initial HUB configuration, a VAX 11/750 with 3 Mbytes of memory, 1 Gbyte of disk storage, two high density tape drives, a floating point accelerator and multiplexers providing 24 asynchronous line interfaces, three Front End Mini (FEM) computers (VAX 11/730), each with 1 Mbyte of memory and 131 Mbytes of disk storage, peripherals for the data-acquisition centre, terminal multiplexer and interfaces for a Cambridge ring local area network, and prototype Data Acquisition Electronics (DAE) and CAMAC modules for the control of instrument components.

The installation of the PUNCH system components has enabled considerable progress to be made on the software necessary for the initial system. The SNS instruments will be controlled via terminals connected to the FEM computers. A program has been written which demonstrates the type of facilities that will be available to the scientist from the terminals and this is being used as a basis for the complete control program. Typically, the scientist sets up his run parameters at the terminal before issuing a variety of commands to start and control the run. At the same time, part of a VDU screen is used to display the status of the instrument. Partially collected data can be read in and displayed on a separate terminal as a further check on the experiment. Once completed, the data will be stored on disk and transferred to the HUB computer via the PUNCH local area network.

The PUNCH Local Area Network (LAN) connects all the FEMs and the HUB computer and provides for data-migration and user-access to the system from terminals located in purpose-built areas, in the newly built data acquisition centre close to the office area, and at the instruments. The LAN is based on a Cambridge ring which can accommodate the extremes of message block size required to satisfy both terminal traffic and fast bulk-data transfers. To deal with the terminal traffic a PUNCH terminal multiplexer has been developed which can provide 16 connections (up to 9.6 Kbaud). The hardware for these multiplexers is SEEL 3012 units. Progress has also been made on fast bulk-data transfer using microcoded interfaces with a basic block size of ~ 2 Kbytes. The present ring includes 6 active nodes linking 6 computers (running under the VMS, RT11 and RSX11M operating systems) and 20 terminals.

A beam line components control and monitoring system to govern the operation of choppers, beam filters and spin flippers and associated electrical devices is being designed and a scheme of cabling the various components around the beam line to the control system in the instrument cabin has been devised.

Sample Preparation and Environment

A certain amount of dedicated laboratory space for scientists to prepare and otherwise characterise their samples will be required. Acceptable locations have been found, a floor plan prepared and an inventory list of apparatus and instrumentation assembled. Rooms have been earmarked for conversion, and design work is under way. Funding-restrictions will probably necessitate some delay in these provisions and the temporary use of alternative accommodation with minimal equipment is anticipated.

Sample environment equipment will be standardised for use on any instrument. Wherever possible, instruments will have sample changers of the same size and all equipment will be controlled by the same type of system. Demand for cryostats, furnaces and sample changers has been estimated from a survey of the user community, allowing a basic set of equipment to be identified for use in the first year of operation. Work on the SNS sample environments has involved the design of a closed-cycle refrigerator sample changer, the construction of a prototype high temperature furnace which has operated up to 2100 K, and the commissioning of a new liquid helium cryostat of the ILL Maxi-orange type. Several User Group meetings have helped to define the requirements for sample environment equipment. On the recommendation of the High Pressure Group, a hydraulic rig for operation to 3 kbar has been ordered. Building of the main sample environment laboratory has been completed.

R & D Towards Pulsed Source Exploitation

Neutron Detector Systems

Scintillator detectors have been successfully built using both the fibre-optic-coded scintillator technique for position-sensitive detectors (PSD) and the sandwich scintillator principle for individual detectors. A module for the High Resolution Powder Diffractometer detector was built using fibre-optic coding. The module is one-eighth of the whole detector which has a 700 mm concentric ring geometry with 20 rings, each 15 mm wide. It has been successfully tested on a laboratory neutron source and is undergoing more detailed tests at the PLUTO reactor, AERE Harwell, using a computer-controlled X-Y table which enables the detector to be scanned across a finely collimated neutron beam.

A more demanding detector system is required for the SNS LOW Q instrument. The main part of this detector has r-θ resolution or 'dart board' geometry. The radial dimension of the resolution elements varies to keep $\Delta r/r$ constant for radii between 5 cm and 35 cm. Azimuthal resolution is 2^0 over most of the area. Methods of adopting the fibre-optic-coded system have been developed using a single layer of glass scintillator 0.5 mm thick coupled to 0.5 mm diameter optical fibres. A small module has been built which incorporates a variety of sizes of scintillator elements to prove the optical coupling and establish a method of assembling the whole detector which will have a total of 5040 elements in 9 identical modules of 560 elements each.

A scintillator detector bank has been installed on the Constant Q spectrometer at the Harwell Linac. This is a bank of 50 individual counters using the sandwich scintillator principle to reduce sensitivity to gamma back-ground. The elements are 10 mm wide and 30 mm high with four layers of lithium glass scintillator each 0.5 mm thick, cemented between 1.5 mm thick non-scintillating glass. A 12.5 mm diameter photomultiplier (PM) is glued directly to one end of the assembly. The intrinsic back-ground count-rate of these elements is about 2 counts per minute and the efficiency for detection of ^{60}Co γ rays is about 5×10^{-6}. This detector bank uses a novel high voltage system in which a single power supply and potential divider is used to control the dynode voltages on all the PMs. Capacitors on the PM bases provide voltage stability over short times and a single variable resistor is used between two dynodes to provide gain control. This arrangement is much more economical than individually controlled power supplies for each PM.

Sandwich scintillators are also being used for the HET high angle detector bank. This system requires detector modules 20 cm long and 6.5 cm wide arranged in concentric rings. A prototype module has been produced using three PMs on each unit optically coupled to the scintillator sandwich by a simple reflecting box. Non-scintillating sandwich materials of both glass and Perspex have been tested with good results. The neutron detection efficiency for neutrons of wavelength 1 Å is over 70%.

A promising development has been made in monitor counters. These are required in the incident neutron beam of a spectrometer to provide a normalising signal for the scattered neutron counts and, in the case of pulsed sources, to measure the incident neutron energy spectrum. The monitor must be radiation hard, and have a very low efficiency for neutrons to avoid saturation, and an even lower efficiency for γ rays. These requirements can be met by a scintillator detector using lithium glass in the form of 0.5 mm cubes distributed over the surface of a thin glass plate on a 5 mm grid. By diluting the scintillator in this way and using in its manufacture ^7Li with only a small proportion of ^6Li, the low detection efficiency is obtained. The glass sheet is placed inside a reflecting cylinder and viewed end on by a 40 mm diameter PM. The device has been tested on the Harwell Linac. The detection efficiency for neutrons of energy 1 eV is estimated to be 10^{-4} and the efficiency for detecting ^{60}Co γ rays is 10^{-7}.

Polarised Neutron Spectrometer

Neutron polarisation analysis is the only method by which unambiguous separation of magnetic, nuclear coherent and nuclear incoherent scattering can be achieved. Many of the techniques associated with polarised neutron scattering are valid only for a monochromatic neutron beam and there is need for much developmental work to extend the techniques for application on white pulsed neutron sources. A developmental polarised neutron spectrometer (POLARIS) has been designed and many of the instrument components have been commissioned or are under construction. A chopper, which will act as the prompt γ-attenuator and provide broad band energy selection of neutrons in the range 3 meV $\leqslant$ E $\leqslant$ 260 meV has undergone extensive tests on the Harwell Linac. Polarisation of the incident beam will be achieved by the resonance absorption technique, initially using polarising filters based on ^{149}Sm. The filters will be housed in a dilution refrigerator and maintained at a temperature of 10 mK. A magnetic field of up to 2.5 T will be available. Filter development work has concentrated on the alloy $SmCo_5$ which is the basis of many permanent magnets. Permanently magnetised polarising filters will operate in the absence of an applied magnetic field thus reducing the complexity of the filter environment and permitting a larger filter area to be used. This is of great importance for a filter used as the analyser on a full polarisation analysis instrument. The POLARIS spectrometer has been designed to facilitate the future development of inelastic polarised neutron scattering techniques such as those based on polarising crystal analysers, and includes the option of a second dilution refrigerator containing a $SmCo_5$ polarising filter to analyse the polarisation of the scattered beam.

Methods of spin-flipping a polychromatic beam have been examined in detail. Particular attention has been given to the development of a Mezei-coil spin-flip chopper which required the magnetic field within the coil to be phased to the SNS pulse and vary with time as t^{-1}. This has been accomplished with an accuracy of better than 0.01% over a time interval which will allow flipping of neutrons with energies up to 1 eV. With a Mezei-coil it is possible to modulate the incident beam polarisation pseudo-randomly. A pulsed source cross-correlation technique based on such modulation has been evaluated. Using this technique it will be possible to convert POLARIS from a total scattering instrument to a mode with full energy and polarisation analysis at all incident and final energies within the capabilities of the polarisers without changing the instrument configuration.

$SmCo_5$ filters have been prepared in the Department of Metallurgy and Materials, Birmingham University. Preliminary neutron-transmission measurements at low temperatures (15 mK $\leqslant$ T $\leqslant$ 200 mK) and low energies (E $\leqslant$ 5 meV) have been carried out at PTB Braunschweig. A full evaluation of one of the filters was performed using a white neutron beam at the Harwell Linac over a range of temperatures between 10 mK and 100 mK. High polarisation (60-90%) was observed over a broad energy band (10 meV $\leqslant$ E $\leqslant$ 140 meV), although the filter transmittance was less than optimal. It is anticipated that higher polarisation and transmittance will be obtained on application of a magnetic field.

Electron Volt Spectroscopy

Pulsed neutron sources are rich in epithermal neutrons and may allow, for the first time, neutron spectroscopy in the

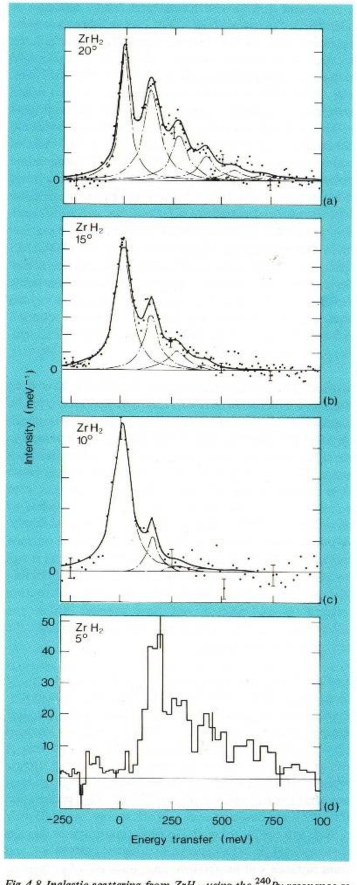


Fig 4.8 Inelastic scattering from ZrH_2, using the ^{240}Pu resonance as an energy analyser, at (a) 20°; (b) 15° and (c) 10°. The curves represent the relative intensity of the inelastic transitions calculated from the simple harmonic oscillator model. (d) Data taken using ^{149}Sm at 5° with elastic scattering suppressed. (83 MB 6053)

electron volt region. New forms of energy analysis are required at these energies and the Laboratory has been involved in developing such techniques. Scattering from many of the systems of potential interest is dominated by a form factor which restricts the cross-section to relatively low values of momentum transfer and so further complicates the problem by limiting useful scattering to the forward direction. Two detection methods, both based on nuclear resonances, are being studied. In the resonance detector method which is being developed in collaboration with Oxford University at the Harwell Linac, the (n, γ) reaction associated with a resonance is used to define the energy of the scattered neutrons. The resultant gamma rays are detected with a high resolution intrinsic germanium detector. In the filtered-beam technique, which was developed in collaboration with Los Alamos, measurements are made with and without a resonance filter in the beam and the difference taken. Fig 4.8 (a-c) shows data from a test experiment where inelastic scattering from ZrH_2 is observed as a function of scattering angle using a ^{240}Pu resonance foil as analyser. A prototype sample-detector chamber has been designed and constructed at RAL (Fig 4.9) and installed at the WNR facility, Los Alamos. Using a double-difference technique and ^{149}Sm as an analyser, inelastic scattering from ZrH_2 has been observed at angles as low as 5° (Fig 4.8d). In these experiments coarse fixed filters were used to improve the elastic/inelastic discrimination. Resonance energy neutrons were removed from the incident beam, eliminating the elastic peak, and secondary filters removed elastically scattered neutrons which would otherwise have been detected at the same time as the down-scattered inelastic signal. These results are very promising and experiments on magnetic excitations are in progress. This spectrometer will be available at RAL for further development work at the SNS.

Single Crystal Diffractometer (SXD)

Efficient and accurate single crystal diffractometry at pulsed neutron sources requires a two-dimensional, position-sensitive detector with uniform response. Such detectors are still in the development phase and SXD will allow this work to continue at the SNS. The position sensitivity of the detector will be of particular interest in the study of phase changes and the satellite reflections associated with incommensurate structures. Outline designs for the instrument have now been completed. The diffractometer will use a 300 X 300 mm^2 position-sensitive Anger camera detector, currently being developed in collaboration with Los Alamos and the Argonne National Laboratory, USA. The detector will be positioned under computer control to cover a range of scattering angles from 20° to 160°. Only one crystal axis will be computer controlled in the initial configuration.

NEUTRON
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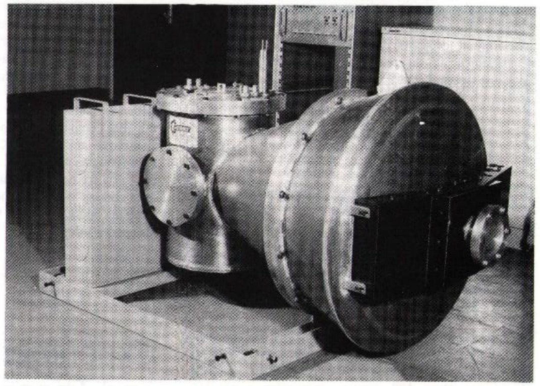
Fig 4.9 The prototype eVS sample chamber and detector assembly prior to being shipped to Los Alamos. (83 RC 3317)



Crystal Monochromators

A feasibility study on the use of crystal monochromators for pulsed source inelastic spectrometers has continued. Measurements at the Harwell Linac have shown the importance of competing reflections in degrading the reflectivities of single crystals. The discrepancies between experimental values and theoretical predictions are partially due to their presence. The measurement of the spectrum transmitted through a single crystal using TOF wavelength sorting is a powerful technique for observing these effects directly. Used in conjunction with a numerical technique developed in collaboration with Southampton University, it is now possible to minimise the loss in reflectivity caused by this effect. Tests on the effect of cooling a Cu crystal monochromator to liquid helium temperatures have shown that gains of a factor of two can be achieved in the reflectivity at energies of 1 eV.

These studies indicate that crystal monochromators are well suited for monochromating incident neutrons up to energies of approximately 300 meV and an initial design study of the proposed Medium Energy Transfer Spectrometer for the SNS, using copper crystals in place of the chopper, has been carried out. This instrument will have a large range of scattering angles which, together with its incident energy range of 20 meV to 160 meV, will make it complementary to HET and TFXA.

A preliminary investigation into the use of magnetically pulsed ferrite crystals as monochromators for pulsed source spectrometers has been performed. Suitably chosen parameters allow the magnetic switching to be phased with the neutron pulse and this reduces the effect of higher order reflections. The possibility also exists of electronically varying the resolution of a spectrometer and thus being able to balance the intensity and resolution parameters to match experimental requirements.

Neutron Choppers

The scientific specification of all the choppers for the first instruments has now been agreed and the engineering design and manufacture of these and their associated drive and control systems is proceeding. The first phase of the collaborative contract with KFA Jülich to develop a magnetic-suspension chopper system was successfully concluded this year with the spinning at 600 Hz of a test rotor for HET. Phase II of this contract has now been placed and will culminate in early 1984 with the commissioning of the operational chopper system for this instrument comprising a family of three interchangeable magnetic-bearing rotors covering the energy range from 100 meV to 1eV at optimum resolution.

Vanadium Scattering

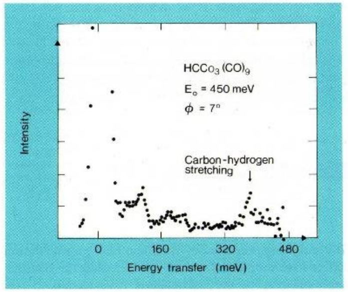
The scattering properties of vanadium on a pulsed neutron source have been calculated numerically using the Gaussian approximation to the multiphonon cross-section. It was found that vanadium behaves as an elastic scatterer to within a few per cent up to energies of 1 eV, with an anisotropy in the scattering of 8%. These calculations allow an assessment of the reliability of using vanadium as a scattering standard to calibrate pulsed source spectrometers.

Current Programme Support

In addition to the research and development programmes, the Laboratory provides support for UK university teams involved in the SERC-sponsored neutron beam scattering programme. Over 100 groups, comprising some 360 university staff, research associates and research students, are supported in the current programme which is based mainly on rented facilities at AERE, Harwell and at the Institut Laue-Langevin (ILL), Grenoble, where the SERC is a partner. Funds for travel, subsistence, materials and equipment for all approved experiments are made available through RAL, which is also responsible for providing assistance with any particular problems arising in connection with experiments, for example in the provision of special apparatus or specialised computing. Over 500 research proposals were submitted for the above facilities during the year; of these 162 have been approved and a further 230 are currently under consideration. 120 visits to ILL were arranged and the transport of equipment and samples to Grenoble was provided on 15 occasions. The figures for ILL are lower than usual, owing to problems with the reactor in the first half of the period. Preparations for university use of the SNS in 1984 have been started and have included a one day Neutron Beam Users' open meeting, held at the Laboratory in September.

With the imminent closure of the old ELECTRIC system on the IBM computer, all supported programs have now been transferred to the new CMS system, usually with small improvements to ease the submission of jobs. The analysis programs are now being used as far away as Strathclyde on data coming over SERCnet from both ILL and Harwell (reactors and Linac). The PRIME continues to be used for interactive work.

Fig 4.10 The inelastic incoherent neutron scattering spectrum of $HCCo_3(CO)_9$. The band at ~ 380 meV corresponds to neutrons which have excited the C-H stretching mode. (83 MB 6054)



Experimental Science and Theory

Chemical Spectroscopy

In collaboration with Durham University, the molecular vibrational spectroscopy of some simple molecules has been investigated by inelastic neutron scattering using the Inelastic Rotor Spectrometer (IRS) at the Harwell Linac and the Filter Difference Spectrometer at Los Alamos. The intensity of the observed vibrational bands varies according to the momentum transfer (ħQ) provided by the neutron. IRS has a detector bank for observing high frequency bands at low Q making it possible to observe very weak oscillators at high frequency (Fig 4.10) and also to follow their intensity with varying Q. A proper analysis shows that even with powder samples this variation of intensity gives information about the magnitude of the atomic vibrational displacements which can be used to constrain normal coordinate analysis calculations, thus contributing to the better estimation of the electron charge distribution.

The Crystal Structure of Li_2MnO_2

A new trigonal phase Li_2MnO_2 has recently been synthesised by prolonged reaction of the spinel $LiMn_2O_4$ with n-butyl lithium. During the reaction, a transformation from cubic to hexagonal close packing of the anions occurs forming a layered structure with manganese on alternate basal planes of the anion array and lithium in the edge-shared tetrahedral sites of the intervening basal planes, as occurs in Li_2VSe_2 (see Fig 4.11). The space group symmetry, determined by X-ray diffraction, is $P\bar{3}m1$ (D^3_{3d}) with lattice parameters

$$a = 3.195(2)\ \text{Å},\ c = 5.303(4)\ \text{Å},\ (c/a = 1.660(2)).$$

As all the Li^+ ions are contained within alternate close-packed layers, this structure has considerable promise as a potential fast ionic conductor. In order to obtain a better understanding of the detailed structural characteristics of Li_2MnO_2, it is necessary to use neutron rather than X-ray diffraction techniques. At present a large sample of Li_2MnO_2 is being prepared in collaboration with Oxford University, for neutron powder diffraction studies.

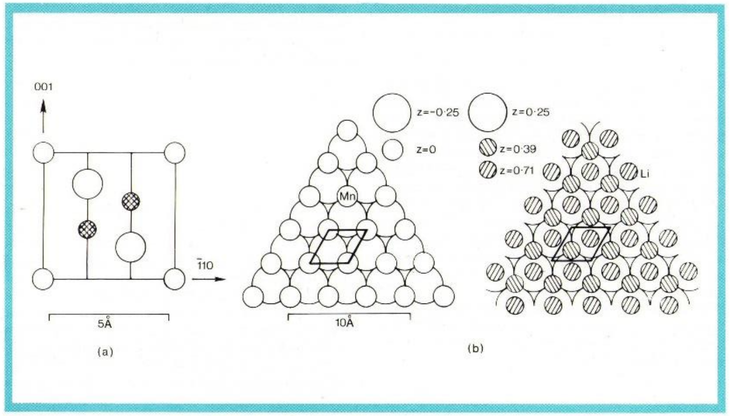


Fig 4.11 The crystal structure of Li_2MnO_2. (a) (1̄10) section (b) successive close-packed layers. Large circles are O^{2-} ions; hatched and open circles are Li^+ and Mn^{2+} ions respectively. (83 MB 6055)

Spin Density of CoGa

The equiatomic intermetallic compound CoGa has some remarkable structural and magnetic properties. The alloy crystallises with the CsCl structure with one sublattice occupied by Co atoms and the other by Ga atoms. However, studies indicate that 16% of the Co sites are vacant and the displaced Co atoms occupy 8% of the sites on the Ga sublattice. Magnetisation, small angle neutron scattering and Mossbauer effect measurements indicate that it is these 'antistructure' Co atoms which dominate the bulk magnetic properties of the CoGa system. The extent of this phenomenon has been clearly and dramatically demonstrated by some recent polarised-neutron measurements of the spin density in a single crystal of CoGa. The experiment was performed at a temperature of 1.7 K and in an applied magnetic field of 4.2 T. Because of the extremely small net magnetic moment of the system (0.07 μ_B at Q = 0) corrections had to be made to the data to account for polarisation of the Co nuclei. The results indicated that while the mean magnetic moment on the Co sublattice is 0.028 μ_B/site, that on the Ga sublattice is 0.039 μ_B/site. It is clear that the moment on the Ga sublattice can only be associated with the Co antistructure atoms, and correction of mean moments at the two sites to account for site occupancies shows that the moment of a Co atom on the Co sublattice is only 0.033 μ_B whereas that of an antistructure atom is over an order of magnitude greater at 0.487 μ_B. Both of these values are well below the value of the Co moment in pure Co metal (1.7 μ_B/atom). Furthermore, the results indicate that the spin distribution is asymmetrical about both the normal and antistructure Co atom sites with 80% and 69% occupation of Eg orbitals respectively. This is again in contrast to the spherical distribution (40% occupation of Eg orbitals) in pure Co. Such behaviour is in accord with band-structure calculations which predict 85% occupation of Eg orbitals.

Dynamical Diffraction in Silicon

Single crystal silicon has a relatively low concentration of defects and is an ideal material for the study of dynamical diffraction effects. In this case it is the amplitude, rather than the intensity, of the scattered and transmitted beams which couples, in contrast to the more familiar kinematical diffraction normally encountered with neutrons. Measurements have concentrated on the observation of the transfer of energy between these two beams which results in a beating of the diffracted intensity known as Pendellösung fringes (the pendulum solution). These fringes were observed as a function of crystal thickness by rotating the crystal slab around the scattering vector on the Badger diffractometer at AERE Harwell's DIDO reactor. This method obviates the need for ultra-precise alignments and is being investigated in collaboration with AERE Harwell as a routine way of examining the defect concentrations in reactor-irradiated silicon.

Micelles

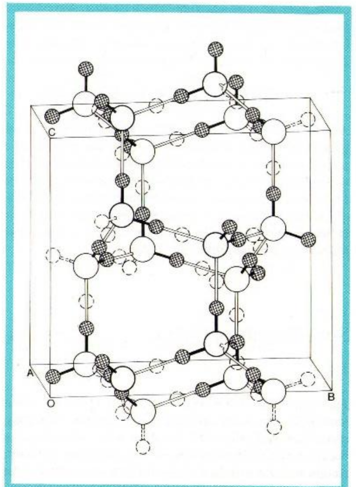
The micellar phase of aqueous surfactants is of technological importance with applications ranging from detergents to pharmacy. In collaboration with ILL, small angle neutron scattering (SANS) has been used to study the internal structure of micelles and the interaction between micelles. A number of cationic and anionic micelles have been studied at concentrations ranging from the critical micellar concentration to the spherical micellar phase boundary. The analysis of such concentrated micellar solutions has been undertaken using a suitable interaction structure factor, calculated for a model potential. This method of analysis is general and can be applied to the study of scattering from any concentrated charged colloidal system. The micelle can be described by a two-shell geometrical model for the variety of charged systems that have been studied. The salient features of the model are a disorganised dry core which need not contain all of the hydrocarbon chain, and a polar region which may be rough, in the sense that its thickness may exceed a head-group diameter. Micelles with trimethyl ammonium head-groups are generally found to be smoother and less hydrated than those with anionic sulphate headgroups.

This work has been extended to investigate the ability of micelles to absorb molecules, which is a particularly important feature of micellar solutions. The analysis of preliminary SANS data for benzene and cyclohexane absorbed into sodium dodecyl sulphate micelles indicates that benzene tends to reside in the outer part of the micelle, displacing solvent to some extent rather than greatly changing the micelle size, and that cyclohexane tends to reside towards the interior of the micelle, expanding the total size without changing the solvation. In both cases increases in aggregation number are only observed at high absorbate concentrations.

Ice

At ambient pressure, ice has a hexagonal structure with each proton randomly distributed between two sites. This disorder becomes frozen-in at low temperatures and the transition to the ordered form is kinetically inhibited. A group at Osaka University has discovered that doping with KOH lowers the kinetic barrier sufficiently to allow the ordered structure to form below 72 K. In collaboration with this group, the structure of the ordered form has been studied using powder diffraction measurements on fully deuterated specimens. Only slight differences in the powder diffraction patterns above and below the transition were found but the symmetry of the low temperature phase was established to be orthorhombic of space group $Cmc2_1$, which is a ferroelectric structure (Fig 4.12). A profile-refinement analysis, however, shows only partial ordering of the protons.

Fig 4.12 The crystal structure of ordered ice. (83 MB 6056)



Condensed Matter Theory

Studies of models of condensed matter have utilised mathematical analysis, computer simulations and numerical computations. The topics include continuing studies of mixed harmonic lattices, classical one-dimensional magnets, polymers and liquid crystals. New topics of research are the response of forced systems, and scattering from magnetic domain walls.

Inelastic Processes

Energetic pulsed fluxes of neutrons from spallation sources will enable many new types of investigations of dynamical structure in molecules and lattices. With this new information will come new vistas and new problems of interpretation.

Forced and Relaxing Systems: The pulsed nature of a spallation neutron source can be used in real time experiments on systems forced by an external field or relaxing towards equilibrium. An analytic study of two models revealed two main features. A curious modulation of line intensities in the inelastic spectra was found as the forcing frequency approached resonance with target transitions, together with unusual commensurability effects, and an additional Lorentzian background to lines in the relaxing case, with a width derived from the coupling of the target to a heat bath. Natural candidates for this sort of study are molecules in a crystal being forced by an external field.

Multiphonon Effects in Lattices: At increasing energy and momentum transfers from the neutron to the lattice, several phonon processes ultimately dominate. Exact numerical calculations of cross-sections show a detailed structure not revealed by approximate treatments which would lead one, erroneously, to surmise 'split-peaks' and other effects. Thus the exact treatment is a caution against approximate analysis in certain regimes. Asymptotic analysis was performed on the scattering law, to see under what circumstances particles eventually appear free.

Powder Averages in Chemical Spectroscopy: The variation of the intensity of a vibrational transition line with momentum transfer provides valuable information that is inaccessible in the alternative optical techniques. When powder samples are used the direction of neutron momentum transfer must be averaged with respect to the molecular frame. A tractable analytic method of doing this has been developed. The method avoids the necessity for either expansion techniques (inaccurate at the energies that make this type of scattering so successful) or numerical analysis.

Scattering from Magnetic Domain Walls and the Confinement of Ultracold Neutrons

Classical ideas can be used to great effect in thinking of the precession of the neutron spin in homogeneous external magnetic fields, for example in the spin-echo technique. In the case of inhomogeneous fields, such as exist near magnetic domain walls or in the confinement of ultracold neutrons in magnetic bottles, it is found that classical ideas can yield the wrong results. This comes partly from the coupling of the centre-of-mass motion to that of its spin. A purely quantum mechanical effect is the nutation of the neutron's spin due to the interference of the incoming beam and the spin-flipped beam, backscattered from a field inhomogeneity.

Polymers

Polymer alloys (blends) are important since a material can often be created with the best properties of each component, for instance toughness and elasticity. A knowledge of thermodynamic and molecular configurational properties is vital in understanding such systems. A theory of neutron scattering to elucidate both aspects was developed. An essential element is the advantage of now being able to interpret experiments at high levels of deuteration labelling of chains, hitherto thought to be ambiguous, thus increasing the speed and accuracy of experiments. The theory was done in collaboration with experimental groups at Imperial College and Oak Ridge, Tennessee.

Liquid Crystals

Phospholipid detergent molecules, the universal components of such bilayers as membranes, form spherical shell assemblies known as vesicles. Within the layers the molecules are orientationally ordered, in a liquid crystalline manner, about a roughly radial direction. Vesicles are an important model for cells and other biological systems as well as having applications, for example in slow drug release. A theory of depolarised light scattering from vesicles was constructed in order to determine structure, ordering and fluctuations. From the transformational properties of spherical tensors and waves, exact results were derived for the effect of collective modes and phase transitions on the scattering.