ISIS status report

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ABSTRACT: We review the progress on ISIS, the pulsed neutron source at the Rutherford-Appleton Laboratory, since the last ICANS meeting. The machine is now running regularly at 100 µA at 750 MeV, and delivering neutrons for an increasing UK and international neutron scattering programme. The current status of the operating and development instruments is summarised, and some examples given of recent science.

1. INTRODUCTION

At the last ICANS meeting in September 1986 (Gray 1987) it was reported that ISIS was running at 550 MeV with 3 x 10^{12} protons per pulse on target at 50 Hz, i.e. a mean current of 24 µA.

ISIS is now running at a peak of over 100 µA at 750 MeV with a fully scheduled set of neutron spectrometers. It has just completed its most successful cycle ever, achieving record peak currents; records of integrated current per day were broken on three occasions, when figures greater than 2000 µA hrs were logged.

This paper gives information on the development of the source, current UK and international usage, and outlines the current state of development of the spectrometers, giving some examples of the science. Detailed reports on ISIS for the two years to March 1988 are given in ISIS 1987 (Rutherford Appleton Laboratory 1987) and ISIS 1988 (Rutherford Appleton Laboratory 1988).

2. REVIEW OF OPERATION

The integrated beam current (µA-hr) per month since June 1986 is shown in Figure 1. In the calendar year 1986, 22,600 µA-hrs were achieved with 121,000 in 1987 and 129,000 µA-hrs so far in 1988. During the month of August 1988, 37,002 µA-hr were delivered to the target (see Figure 2). The highest average current over one day in August was 84 µA with the peak at just over 100 µA. This maximum average daily current was increased to 86 µA over 24 hours in September. Over the month of August, the average current was 56 µA. There were two two-day shutdowns caused by equipment failure. The run continued until 15 September.

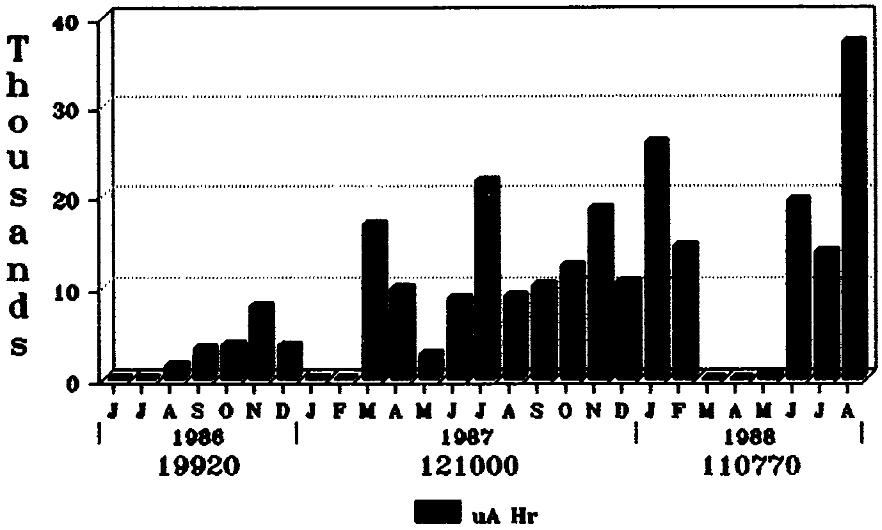


Fig. 1 Integrated ISIS beam current in µA hrs from June 1986 to date.

During 1987 there were two successful target changes. These are discussed more fully in a paper by A Carne at this meeting. The failure is believed to be caused by swelling of the depleted uranium as a result of repeated thermal shock. After the failure of target number 2, the control system which protects the accelerator and transfer lines against abnormal lost beam pulses was modified and refined. This resulted in the number of temperature shocks to the target being reduced by more than a factor of 10 in a given time. Target number 3 has taken 129,000 µA-hrs and is still mechanically sound. Of the lost time on the facility during 1988, 21% is due to failures in the injector system, 2% in the extraction power supply and 1.3% in the synchrotron RF system.

Experience with running at 100 µA has resulted in a weekly scheduled stop of one 8 hour shift to change the H^- ion source and to change the filters in the methane moderator system. This stop accounts in significant part for the 7 day periodicity visible in Figure 2. This arrangement will be reviewed as more experience is gained. The available resources above those required for operation are being used to improve the reliability of operation at 100 µA rather than to increase the operating current.

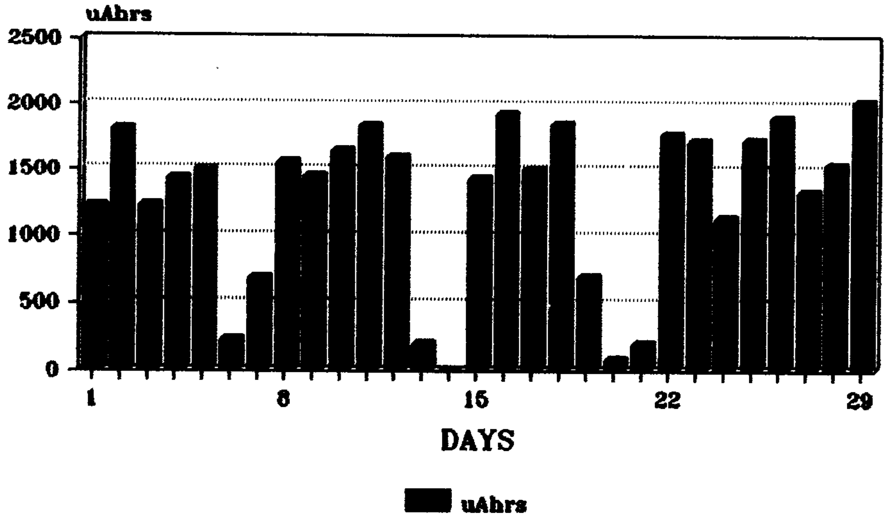


Fig. 2 Integrated beam current in µA hrs delivered to the target during cycle 4, 1988.

At 100 µA (1.25 x 10^{13} protons per pulse), typical beam transfer efficiencies during routine running are :

efficiency	98-99%
Trapping efficiency in synchrotron	86%
Acceleration efficiency	99%
Extraction and transfer to target	99%

The lost beam collector system continues to work well. The system concentrates beam lost at injection at trapping into collectors with suitable materials and which are removable.

Induced activity on synchrotron components leads to radiation levels on contact of 100,000 µSv/hr at the collectors but of only 250 µSv/hr in most of the rest of the synchrotron.

It is noticeable that the machine vacuum has not been let up since the shutdown in May.

3. BEAM TIME DEMAND AND SCHEDULING

During 1987 and 1988, a total of 1940 days of beam time was allocated for user experiments on between 5 (early 1987) and 10 (current) instruments; with 4310 days requested, this represents an average oversubscription factor (days requested/days available) of 2.2. The distribution between the three allocation rounds is shown in Table 1. Table 2 gives the allocation data by instrument for round 1/88. On the fully scheduled instruments, oversubscription factors range between 1.1 and 3.2.

4. INTERNATIONAL PARTICIPATION

In round 1/88, UK users accounted for 64% of the scheduled beam time. Figure 3 shows how the non-UK component was distributed by country. Italy, France, West Germany and Sweden together accounted for 73% of the non-UK time, the remainder being largely taken up by users from the Netherlands, USA, India, Japan and Spain.

Bilateral use agreements are at an advanced stage of negotiation with Italy, France and Sweden. A four-year agreement with the Netherlands has been signed. Four countries have been or are involved in the construction of neutron instruments, including India (Be filter on the early IRIS spectrometer), Italy (the PRISMA spectrometer), Japan (the multi-angle rotor inelastic instrument MARI). A rotating analyser instrument (ROTAX) will be developed by the University of Würzburg, and a draft agreement relating to this is at the advanced negotiation stage.

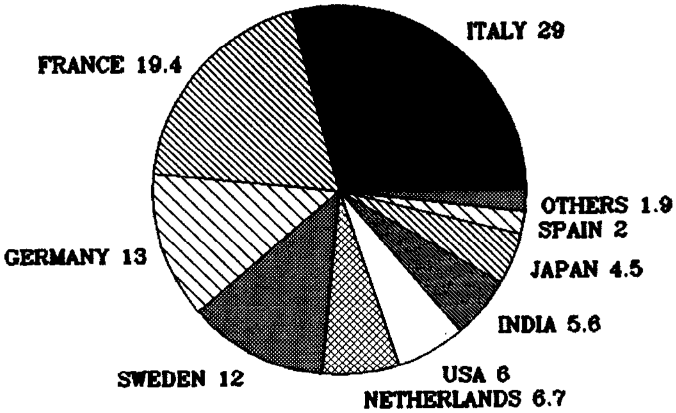
TABLE 1

Round	Days Available	Instrument Days Requested	Instrument Days Allocated
1/87	143	965	591
2/87	71	1439	392
1/88	120	1906	957
TOTALS 1987 + 1988	334	4310	1940

TABLE 2

ROUND 1/88

Elastic Spectrometers	Days Requested	Days Allocated
HRPD	241	102
LAD	210	103
CRISP	220	100
LOQ	159	100
(POLARIS	91	67)
Inelastic Spectrometers		
HET	249	95
TFXA	103	92
IRIS	325	100
(eVS	76	104)
	1674	863
Muons		
μSR	232	94
	1906	957



FOREIGN USE

Fig. 3 Distribution of non-UK use of ISIS beam time by country for round 1/88.

5. SCHEDULED INSTRUMENTS

As indicated in Table 2, nine neutron instruments are now being scheduled, together with the µSR line. Two further instruments are in the commissioning phase (SXD and PRISMA), and three under construction (SANDALS, MARI and ROTAX). KARMEN - the Karlsruhe-Rutherford medium-energy neutrino experiment - has had 1/9 of its detector installed, and is undergoing test. Of the 18 available beam holes around the target station, 13 have been taken up. In addition, a test beam facility has been installed on the methane moderator; its initial use will be for resonance radiography development and detector tests.

Table 3 lists the characteristics of both currently-scheduled and development instruments. The major changes to the various instruments since 1986 are as follows.

(a) Elastic Instruments

HRPD In 1986 at the time of ICANS-IX, only two of the eight octants of the backscattering bank had been installed. Currently, six are in place, resulting in significant increase in throughput and expansion of the scientific programme. A low angle bank gives access to d-spacings up to about 50Å, and construction of a 90° detector bank for restricted sample environment work (especially pressure) is in hand; a temporary detector module is being used in initial 90° tests.

Although HRPD is classed as a powder diffractometer (which has been used extensively in key high T_c superconductor experiments), its uniquely high resolution has opened up other exciting areas, through its ability to see fine details in line profiles. Examples include residual stress analysis in engineering components, observing variable oxygen stoichiometry in the warm superconductor $YBa_2Cu_3O_{6+x}$, domain structure changes close to phase transitions (e.g. the ferroelastic transition in $LaNbO_4$ - see Figure 4), and periodicities in cycloidal magnetic structures (the 760Å repeat in $BiFeO_3$ could be seen after only a few seconds exposure time (Figure 5)). Ab initio structure determinations from powders are becoming semi-routine; recent examples include the high temperature α-phase of malonic acid, and methylamine deuteroiodide CD_3ND_3I. Unit cell parameters can be refined to 5 parts in 10^6, and the instrument is capable of observing inhomogeneties in well-recognised "standards"!

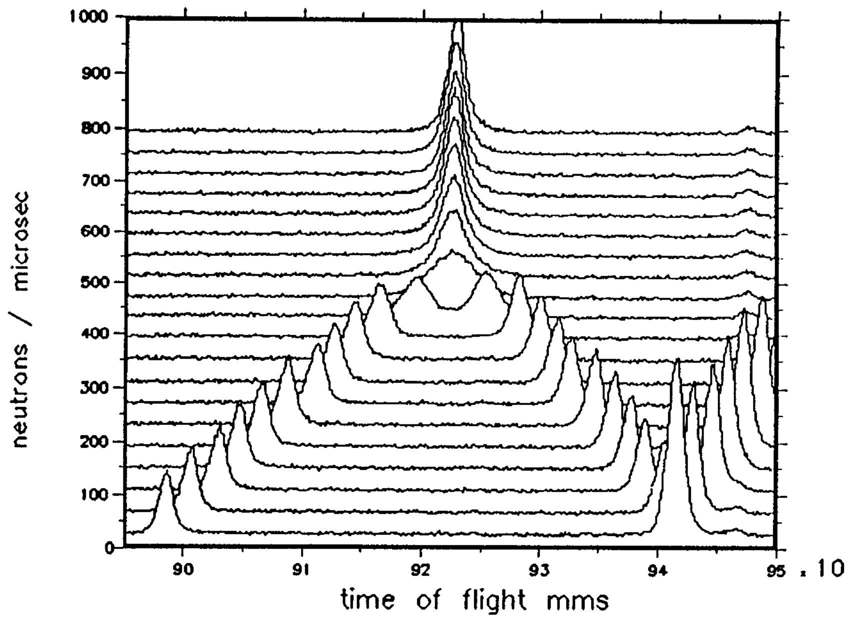


Fig. 4 Scans through the ferroelastic transition of lanthanum niobate at temperature intervals of 10. Not only is the transition well-defined, but detailed peak-shape analysis shows the formation of needle-shaped domains.

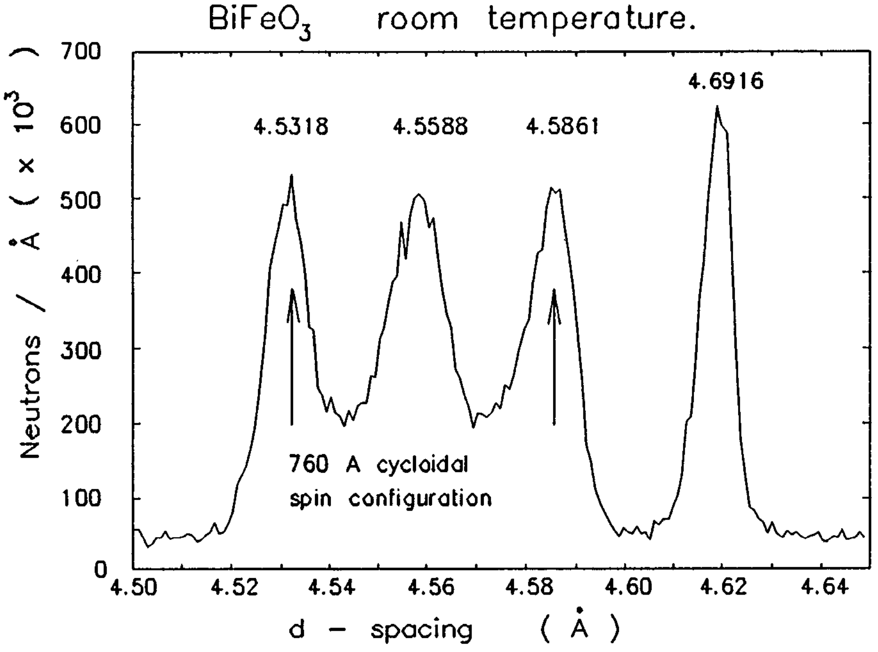


Fig. 5 The 760 Å cycloidal spin configuration splitting in $BiFeO_3$.

TABLE 3

INSTRUMENTS AT ISIS

ELASTIC

HRPD	High-resolution powder diffractometer	Ab-initio structure determination, large unit cell structure refinement, phase transitions, mixed phases, line broadening, high-pressure studies	$\Delta d/d \sim 5 \times 10^{-4}$ (backscattering) $\Delta d/d \sim 0.1$ (low angle bank) guide: $\lambda^* = 0.98$Å minimum wavelength = 0.5Å.
POLARIS	High intensity powder diffractometer	Magnetic structures, phase transitions, kinetic studies, small samples, high pressure work	$\Delta d/d \sim 5 \times 10^{-3}$ (backscattering) $\Delta d/d \sim 8 \times 10^{-3}$ (90°) $\Delta d/d \sim 2.5 \times 10^{-2}$ (forward scattering)
LAD	Liquids and amorphous diffractometer	Structures of liquids and amorphous solids, medium resolution powder diffraction	$0.5 < Q < 100$ (Å^{-1}) $\Delta Q/Q = 0.004$ (backscattering)
SANDALS	Small angle diffractometer for amorphous and liquid samples	Static structure factors of fluids, amorphous materials and biological systems	Minimises inelastic corrections: $2\theta_{max} = 120°$, $\lambda_{max} = 6$Å $\Delta Q/Q \sim 0.01-0.04$,
SXD	Single-crystal diffractometer	Single crystal structure determination study of structural phase changes and magnetic order, reciprocal space surveying	$0.2 < Q < 30$ (Å^{-1}) 1.2-300K accessible, position sensitive detector.
CRISP	Pulsed source neutron reflectometer for surface studies	Surface structure, interfaces and surface magnetism	Resolution (in $\Delta\theta$) 2-10%; Q range 0.01-1.3 Å^{-1} using 0.5-6.5Å wavelength neutrons; inclined beam for liquid surfaces.
LOQ	Low-Q diffractometer	Macromolecular, biological and other large scale structures	$0.005 < Q < 0.2$ (Å^{-1}), $\Delta Q/Q \sim 0.05$

INELASTIC

HET	High-energy transfer spectrometer	Magnetic and vibrational excitations single particle motion in quantum systems	Chopper; incident energy 50-2000 meV ε range 20-1000 meV 1% energy transfer resolution.
MARI	Multi-angle rotor instrument	Dynamic structure factors of liquids and magnetic systems, inelastic excitations in crystalline amorphous and disordered systems, molecular spectroscopy, momentum density	Chopper; incident energy 20-1000 meV ε range 10-500 meV 1% energy transfer resolution ϕ = 3-135°.
TFXA	Time-focused crystal analyser	Inelastic scattering from magnetic and vibrational systems, especially molecular spectroscopy of hydrogenous systems	hω range 2-1500 meV ~ 1.5% energy transfer resolution, elastic line width 0.2 meV.
IRIS	High-resolution quasielastic and inelastic spectrometer	Rotational and translational diffusive motion in atomic and molecular systems, quantum tunnelling, crystalline electric field transitions and low lying inelastic modes	Graphite analyser (002) reflection: 15 μeV resolution at E_a = 1.83 meV Q = 0.25-1.85 $Å^{-1}$ (004) reflection: 50 μeV resolution at E_a = 7.2 meV Q = 0.5-3.7 $Å^{-1}$
eVS	Electron-volt spectrometer	Momentum density studies in low mass systems	Resonance analysers being developed in the range 1-20 eV
PRISMA	High-symmetry coherent inelastic spectrometer	Phonon and magnon collective excitations in single crystals	16 independent crystal analysers, 3-axis analogue
ROTAX	Rotating analyser crystal spectrometer	Structural and magnetic excitations in single crystals	One rotating Ge analyser, position sensitive detector

HRPD is a very powerful instrument for a wide variety of materials science work. Apart from powder samples, it has potential new uses on single crystals, and tests on its potential in high-resolution inelastic mode are planned.

<u>LAD</u> The original gas detectors in this liquids and amorphous materials diffractometer have been replaced by Li glass scintillator in the 20°, 35°, 58° and 90° positions. The consequent count rate increase of about five has resulted in an expansion of isotope substitution first difference work (e.g. aqueous $Cu(NO_3)_2$ with nitrogen substitution, chromium perchlorate with chromium substitution). Work on the instrument has also expanded to gaseous systems, and an experiment on gaseous deuterium near the critical point having recently been completed. The very high Q capability continues to be capitalised on, a recent experiment on vitreous GeO_2 showing clear structure in S(Q) out to 50 $Å^{-1}$.

<u>POLARIS</u> The direction of polarised neutron work has recently been reassessed at ISIS, with more emphasis being placed on the possible use of polarising mirrors. POLARIS is consequently being reequipped as a medium intensity powder diffractometer, with three detector banks (low angle $\Delta d/d \sim 2.5 \times 10^{-2}$, high angle $\Delta d/d \sim 5 \times 10^{-3}$, and a 90° bank for restricted sample environment work $\Delta d/d \sim 8 \times 10^{-3}$). The initial complement of detectors was installed within the last week, and commissioning tests are taking place. To give an idea of the kind of data we expect to obtain, Figure 6 shows patterns for an Al_2O_3 standard at the 150° and 90° detector positions for a single detector after 24 minutes running on a 1 cm^3 sample. With all detectors in place, data of this quality will be obtained in around 2 minutes. This gives the potential for up to 10^5 simple experiments per year.

<u>CRISP</u> This is a critical reflection spectrometer that has been constructed and commissioned since the last ICANS meeting. Using an incident beam inclined at 1.5° to the horizontal, it probes the density profile of interfaces in the direction normal to the interface. Reflectivities of 10^{-6} are obtained routinely; recently, reflectivities down to 10^{-7} have been achieved, extending CRISP into a region which is crucial for discriminating between competing models of particular interface structures. Figure 7 shows the kind of data obtained from an 1185Å deuterated Langmuir-Blodgett film deposited onto a silicon wafer: the continuous line indicates the theoretical model.

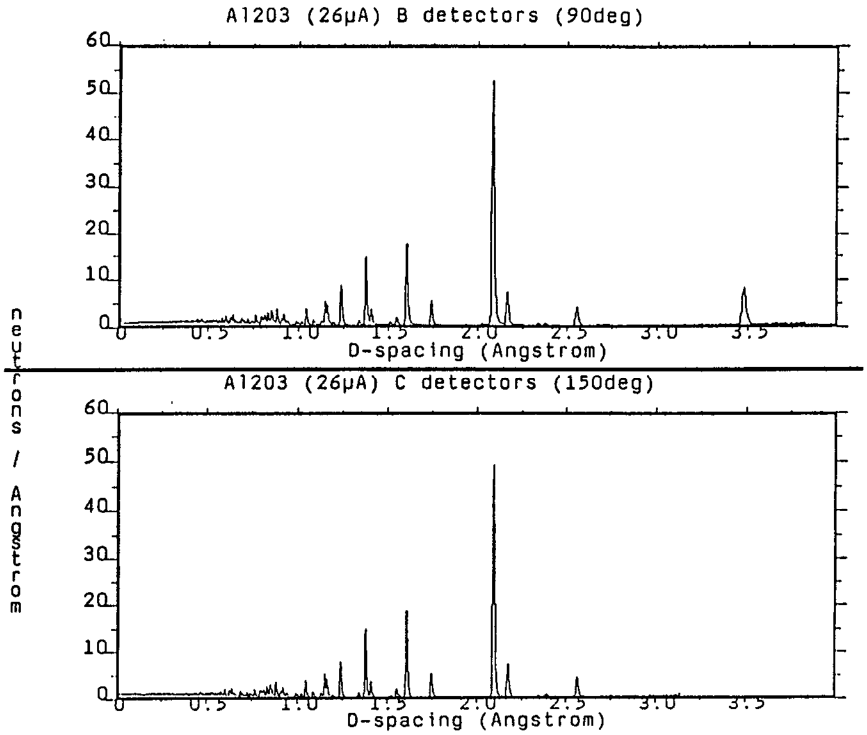


Fig. 6 Test run on POLARIS of a 1 cm^3 Al_2O_3 standard, showing data obtained at the 90° and 150° detector positions. With all detectors in place, such spectra will be obtainable in about 2 minutes.

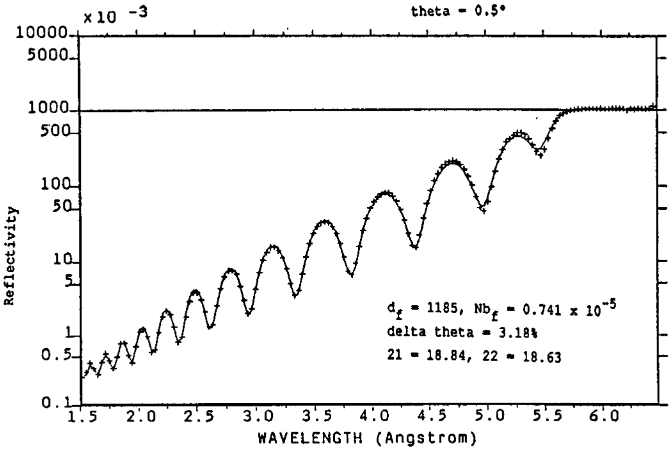


Fig. 7 Reflectivity measurements on an 1185 Å deuterated Langmuir-Blodgett film on silicon; the continuous line indicates the theoretical model (R. M. Richardson).

The versatility of, and demand on, this instrument is illustrated by the very wide ranging nature of its scientific programme in surface chemistry, solid films, and surface magnetism. A high proportion of the demand is from industrial users tackling problems with complex systems. A recent example concerned adsorption at the air solution interface of <u>mixed</u> surfactants, using selective deuteration to determine relative composition and structure.

A resistive wire, one-dimensional multidetector, active area 200 x 40 mm^2, with a positional resolution of ~ 0.9 mm in the long dimension, has recently been successfully tested. This will allow studies to be extended to the diffuse non-specular scattering from interfaces.

<u>LOQ</u> The low-Q diffractometer, designed for investigating macromolecular, biological, and other large scale structures, has been reconfigured. The moderator to sample distance has been reduced from 16 to 11.4m, with a resultant increase in flux, and allowing 25 Hz operation using one chopper. Frame-overlap mirrors remove frame overlap contamination above 12Å. A BF_3 multiwire area detector is installed 4.3m from the sample. A Q range of 0.005-0.25 $Å^{-1}$ is accessible, allowing size ranges of 20-1000Å to be probed in a single experiment.

The user programme on LOQ - as would be expected of such an instrument - is wide ranging over macromolecule studies, colloid science and materials. Figure 8 shows data from shear-flow-aligned micelles of 1% $C_{16}E_8$ in 0.5M Na_2SO_4 at 30°C, parallel and perpendicular to the long axis of the micellar rods. An example of materials science work is the study of precipitate formation and growth in aluminium-lithium alloys which offer substantial weight savings over existing alloys for engineering structures. These studies showed how small amounts of Cu and Mg modify the precipitate, which is thought to be a significant cause of embrittlement of these alloys with ageing.

<u>SXD</u> Rapid progress has been made on this development instrument over the last few months, largely due to the successful initial testing of a new ZnS position sensitive detector module with 5 mm resolution. The low γ-sensitivity of the ZnS scintillator has allowed the detection of very high $\sin\theta/\lambda$ reflections; this is illustrated in Figure 9 where the (0024) of SrF_2 (d = 0.24Å) is clearly observable with the detector at 90°. The comparison with Li glass scintillators is self-explanatory. Other tests have demonstrated the ability of this detector to survey reciprocal space with the examination of one-phonon thermal diffuse scattering in SrF_2: hitherto unseen features in the TDS behaviour have been observed.

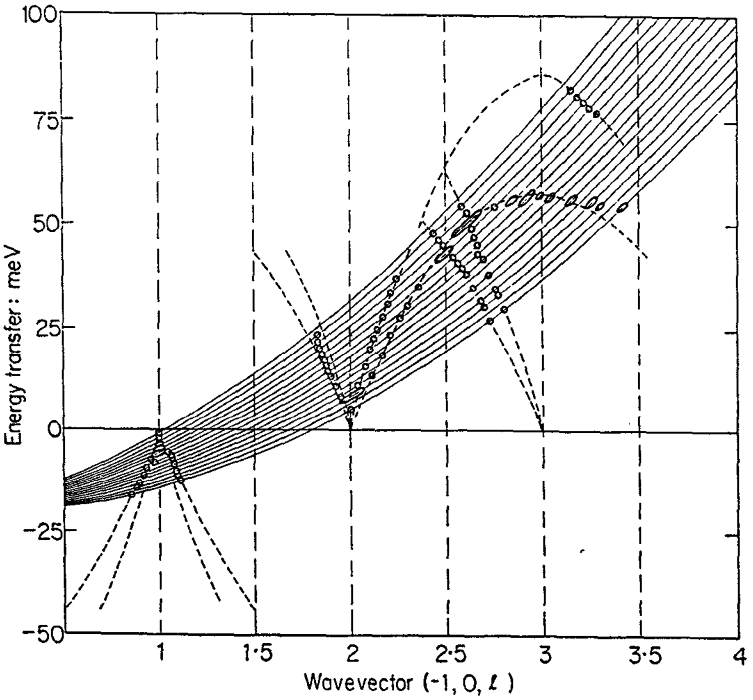


Fig. 8 Q⊥, Q|| intensity plots for 1% $C_{16}E_8$/0.5 M Na_2SO_4 at a shear gradient of 5000 s^{-1} at a temperature of 30°C (J. Penfold, P. G. Cummins, and E. J. Staples).

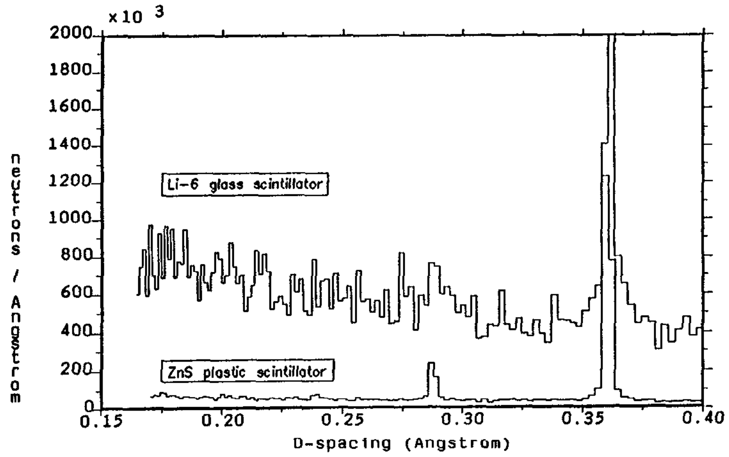


Fig. 9 Test measurements on SXD on a single crystal of SrF_2, comparing results from the test ZnS detector module with that from Li glass scintillator. The 0024 at a d-spacing of 0.24 Å is just visible in the low-noise ZnS spectrum.

Test work is proceeding on a variety of crystals, including some with large unit cells, to assess the feasibility of high resolution measurements on such crystals. The relatively low cost and ease of manufacture of ZnS modules are expected to result in a 300 x 300 mm^2 detector with 3 mm resolution. Once this has been commissioned, regular scheduling of SXD will follow, hopefully in mid 1989.

(b) Inelastic Instruments

As these will be dealt with in more detail in the paper by Andrew Taylor, my comments will be restricted to brief summaries of major modifications and developments.

On HET, the 10-30° 2.5m intermediate angle range detectors have been upgraded with 256 ^3He tubes, and a new chopper slit package has extended the incident energy available down to 50 meV. Two scientific highlights include measurements of the highest-ever observed magnetic excitation ($^3H_4 \rightarrow {}^3F_4$ at 809 meV in Pr metal) and the first successful single crystal experiment on HET of spin waves in cobalt, where measurements were made out to the zone boundary (~ 300 meV). On the time focused crystal analyser spectrometer TFXA, the analyser efficiency has been doubled by using thicker crystals with a more relaxed mosaic spread. The instrument is optimised for the study of vibrational dynamics of hydrogenous samples, recent particularly exciting work including studies of a hydrodesulphuration catalyst (MoS_2). On the high resolution quasielastic and inelastic spectrometer IRIS, resolution has been enhanced with the installation of a pyrolytic graphite analyser.

The development programme on the electron volt spectrometer eVS was fully reassessed during 1988. The resonance detector analyser programme was suspended, and other options are now under consideration. A momentum density user programme has started on eVS, and an intermediate angle bank has been installed.

The study of coherent excitations in single crystals is an area that has been very successfully exploited using triple axis spectrometers on reactor sources. Dispersion curve measurements on ISIS are made using the new PRISMA instrument. This operates in inverted geometry, with the final energy of the scattered neutrons analysed by 16 individually-movable analyser-detector arms.

Under an agreement between SERC and the CNR Frascati, PRISMA was provided by Italy for installation on ISIS. The components arrived at RAL from Italy in mid-1987, and the instrument was installed on ISIS. Within the past few weeks, initial data of impressive quality have been obtained, showing clearly the power of this instrument to measure dispersion curves. Figure 10 shows the sections in (E,Q) space cut by each of the 16 analysers for a single crystal of Be, while Figure 11 shows the results for one analyser, underlining the excellent signal/background obtained. From such sections, the phonon dispersion curve can be constructed, as on Figure 10, where the known dispersion curve is plotted as dotted lines. These results were obtained in only 600 µA hours, equivalent to about 6-7 hours at current running. In the more complex $KTaO_3$, a good quality dispersion relation was obtained in a single day. The potential of PRISMA for phonon dispersion curve measurements is clear. The instrument will be officially inaugurated at a ceremony on 4 November 1988.

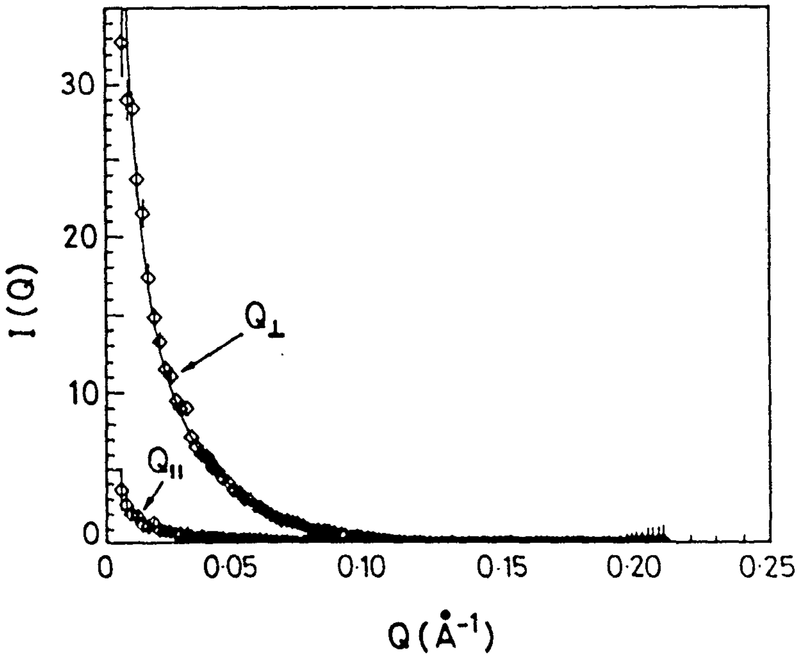


Fig. 10 Dispersion relation measurements on a single crystal of beryllium obtained during early tests of PRISMA. The solid lines are the cuts in (E, Q) space made by each detector, while the dotted lines demote the known dispersion relation.

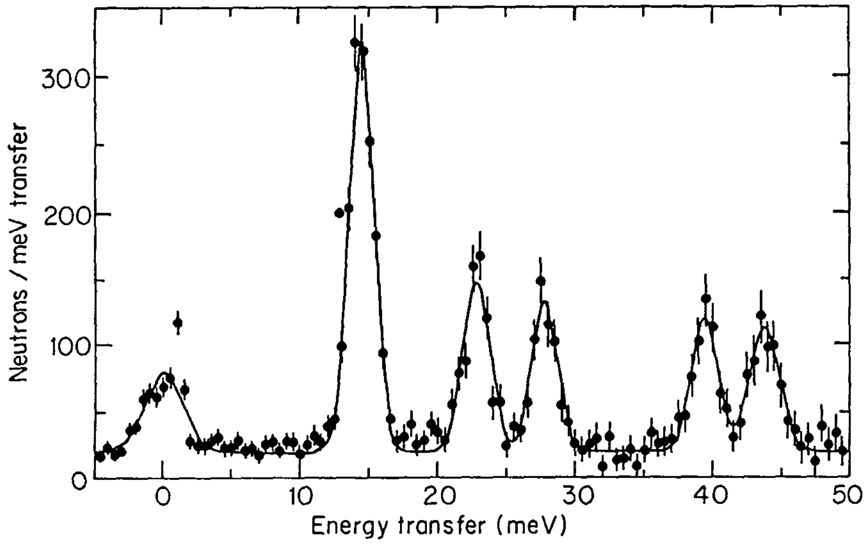


Fig. 11 Measurements taken from one analyser of PRISMA on the same Be crystal as Fig. 10. Figure 10 is constructed from several such scans.

6. SUMMARY

ISIS is now running regularly at around 100 μA currents at 750 meV. Nine neutron instruments and the μSR line are being regularly schedueld, with increasing demand for an increasingly sophisticated user community in the UK, Europe and elsewhere. With this regular running, the capabilities of such a high intensity pulsed source are increasingly resulting in new science in both elastic and inelastic scattering studies. Several further instruments are under development and construction, with the first scheduled experiments on three of these expected during 1989. On the machine side, priority is being given to further improving reliability before the next stage in increasing the current to 120-130 μA.

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