

HARWELL LABORATORY

NEUTRON SCATTERING

INSTRUMENTATION

AND

ANCILLARY EQUIPMENT

FOR SALE

Contents

Following the closure on 31st March 1990 of the two Harwell MTR's, PLUTO and DIDO, AEA Technology is offering the neutron scattering instruments and some ancillary equipment for sale. This brochure gives specification of the instruments and examples of their use.

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July 1990

## 1. Harwell's Neutron Beam Instrumentation

The instruments in Harwell's two reactors PLUTO and DIDO were installed during the 1960's and 1970's, but nevertheless have been subjected to a number of improvements during subsequent years. They have proved reliable work-horses, which were nearly all in full use until the shutdown on 31st March 1990. They have contributed to a large number of publications over the years ( $\sim 380$  since 1977), and much commercial work has been carried out using them over recent years.

The instruments are accommodated on 7" diameter tangential beam tubes passing through the  $D_2O$  reflector tank in the PLUTO reactor, and on 4", 6" and 10" radial beam tubes in the DIDO reactor. Both reactors operated at  $\sim 25MW$  giving  $\sim 1.5 \times 10^{14}$  n/cm<sup>2</sup>/sec neutron flux. They were both heavy-water moderated and cooled, graphite reflected and helium blanketed, with secondary cooling by light water and cooling towers.

The interfaces to the controlling computers is via CAMAC or a micro processor unit. All are currently run from DEC computers: VAX, PDP11 and PDP8's. At the time of shutdown these were in the process of being changed to IBM Compatible PC's, and it is envisaged that this change would be incorporated into any instrument sold-according to customers wishes.

The instruments are offered for sale, with possible options:-

- 1) As seen, at the Harwell gate
- 2) Relocated on a customers reactor
- 3) Relocated with modifications/improvements
- 4) With the addition of commissioning and training of users.

Ancillary equipment for sale is listed at the end of the brochure.

Potential customers should consider:-

- (i) Their requirements
- (ii) How these instruments will satisfy these as seen or modified
- (iii) Will the instrument fit the space available, particularly regarding height clearance above the floor, and overall area.

Diagrams can be supplied on request to aid these considerations.

The expertise in operation and data analysis built up at Harwell over the years is offered on a consultancy basis to help train new users of the instruments as required.

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SALE OF ITEMS:- It is intended to sell complete instruments and major items by tender. Details of the tender exercise will be made available. They can be obtained from the above address.

## NOTE ON NEUTRON SCATTERING TECHNIQUES

Neutrons have proved to be an immensely useful tool for the investigation of many aspects of condensed matter physics, chemistry, biology, materials science and even technology-engineering. They have played an exceptional role in the understanding of collective excitations of crystal lattices and magnetic systems, and of the detailed elucidation of many subtle aspects of second order phase transitions.

What makes the neutron so useful?

1. It can probe both the spatial and temporal nature of excitations at the same time. The wavevector range ( $\sim 0.0001\text{\AA}^{-1}$  to  $50\text{\AA}^{-1}$ ) and corresponding energy range (1meV to 1eV) of fluctuations in materials which it can probe correspond to just those of the excitations, collective or critical, in solids.
2. Its penetration into most metals is good (5cm steel, 10cm Al) - so that bulk average properties, or spatial profile of properties, can be measured; in situ experiments can be made easily at low and high temperatures (1mK to 3000K), high pressures, and high magnetic fields; little sample preparation is necessary.
3. The scattering cross section is relatively weak, allowing accurate theoretical (first Born approx.) and experimental evaluation to be made and absolute values to be determined.
4. The scattering lengths of elements vary randomly with Z, and are roughly of the same order of magnitude - enabling positions of light atoms to be determined.
5. Both coherent scattering, giving information on the correlated behaviour of different nuclei (atoms), or incoherent scattering, giving information on the behaviour of individual nuclei (atoms), can be observed.
6. Isotopic substitution can be used to vary cross sections and identify scattering processes.
7. The form factor for nuclear scattering is unity - enabling large Q and therefore good resolution to be obtained.
8. Magnetic scattering can be observed from magnetic elements (and nuclei) enabling magnetic structures and excitations to be probed.
9. Little or no radiation damage to sample.

### Disadvantages

- We need a high flux source - reactor, or spallation source.
- The sample must be relatively small ( $< 50\text{cm}$ ).
- The experiment is slow (costly) - but very informative.

### Unique Areas of Information

1. Magnetic scattering - structure, excitations, spin densities.

2. Energy-wavevector dependence of excitations. Phonons and Magnons
3. Energy-wavevector dependence of critical fluctuations at phase transitions.
4. Use of polarised neutrons to gain extra information - eg. isolation of magnetic scattering.
5. Use of isotopic substitution to identify scattering.
6. Use of incoherent scattering to gain information on dynamic behaviour of individual atoms.
7. Crystal and amorphous structures - position of light elements, good resolution (high Q).
8. Biological samples - little radiation damage.
9. Measurement of stress in depth into metallic components.
10. Measurement in 'extreme' in situ environments low and high T, high P, high H.
11. SANS to obtain good volume averages of size, shape, and volume fraction of inhomogeneities in materials of (1-1000 nm), making use of all advantages of neutrons; particularly H-D isotopic substitution.
12. Neutron Spin Echo Techniques - very high energy resolution.
13. Neutron Optics Technique - fundamental physics.

#### DEFINITIONS

The following definitions apply to terms used in the notes on the instruments:-

Neutron momentum  $\hbar k$  is related to wavelength and energy by the following:

$$k = \frac{2\pi}{\lambda} \quad E = \frac{\hbar^2 k^2}{2m}$$

where  $\lambda$  is the wavelength and  $m$  is the neutron mass,  $k_i$  and  $k_f$  are the incident and scattered wave vectors. The scattering vector  $Q = k_i - k_f$  and the neutron energy loss is  $\hbar\omega = \hbar\nu = E_i - E_f$ , where  $E_i$  and  $E_f$  are the incident and scattered neutron energies.



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HARWELL NEUTRON SCATTERING INSTRUMENTS FOR SALE

A. PLUTO

<u>Hole</u>	<u>Instrument</u>	<u>Abbreviations</u>
7H1R	Small Angle Neutron Scattering	SANS
7H4R	Powder Diffraction	PANDA
7H2R	Double Back Scattering Diffractometer. MARX, or 3-AXIS.	DBSD, MARX/3-AXIS
7H2L	Triple-Axis Spectrometer	PTA

B. DIDO

6HGR9	Radiography	THERMAL
6H1	Radiography	COLD
10H	Powder Diffractometer	HRPD
4H1	Powder Diffractometer	CURRAN
4H2	Single Crystal Diffractometer	MK VI 4 Circle
4H2	Single Crystal Diffractometer	MK VI 2 Circle
10H	Triple-Axis Spectrometer	DTA

## TYPICAL USES FOR NEUTRON SCATTERING INSTRUMENTS

### SANS

Heterogeneous materials-cements, microstructure of alloys, sols and gels, clays, and other porous media.

### PANDA

Powder Diffraction-structure and phases stress measurement in weldments and components.

### DBSD

Stress measurement in weldments and components, also inelastic scattering in MARX or 3-axis mode.

### PTA

Diffuse and inelastic scattering from single crystal of ordered and disordered materials.  
Stress measurement.

### RADIOGRAPHY-THERMAL

Rolls Royce Blades, Fuels etc.

### RADIOGRAPHY-COLD

Live radiography, PWR Reflooding.

### HRPD

Powder diffraction structure and phases, liquid diffraction.  
Stress measurement.

### CURRAN

Powder diffraction, structure and phases. Liquid structures.

### MK VI 4 CIRCLE

Single crystal structure; Texture, Stress.

### MK VI 2 CIRCLE

Single crystal structures, magnetic diffraction; Phases.

### DTA

Diffuse and inelastic scattering from single crystals of ordered and disordered materials.



# DIDO

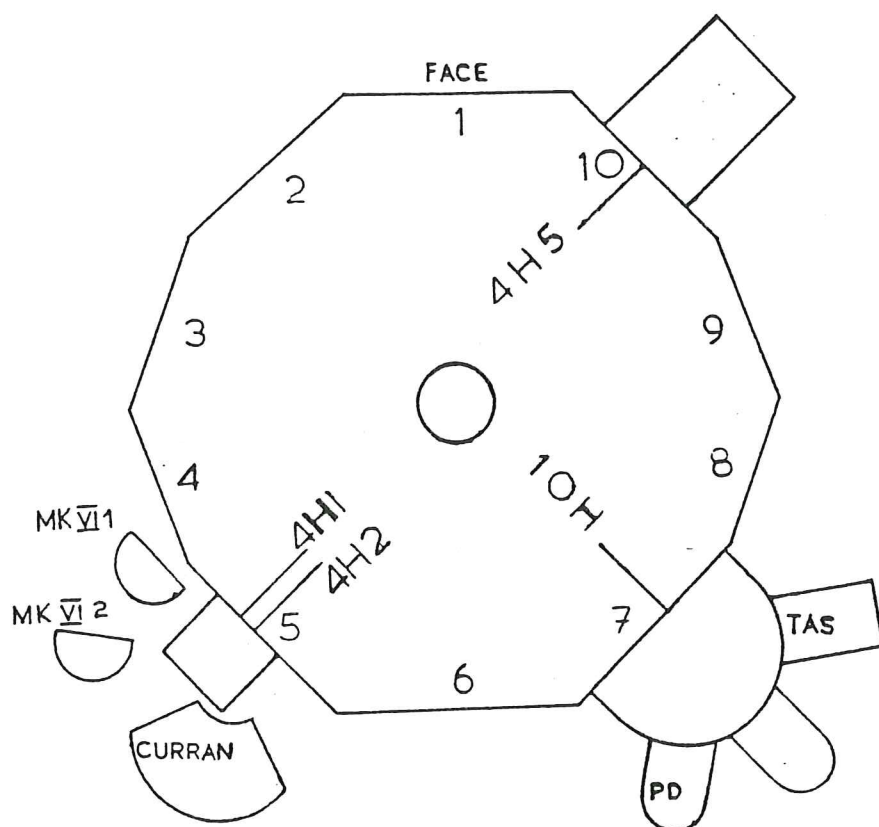


Figure 1.

## DIDO instruments

4H1	Mk.VI 1	4 circle diffractometer
	Mk.VI 2	2 circle diffractometer
4H2	CURRAN	CURRAN powder diffractometer
10H	PD	2 axis powder diffractometer
	TAS	Triple axis spectrometer

# PLUTO

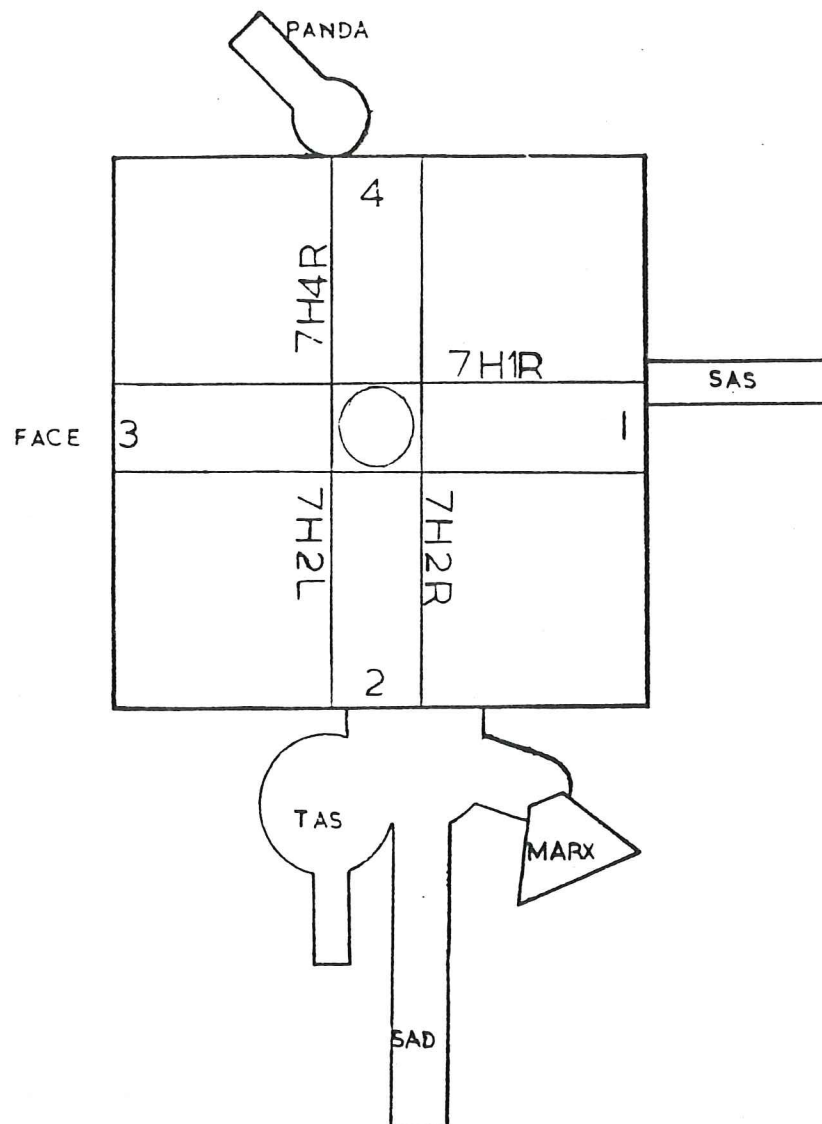


Figure 2.  
PLUTO instruments

7H1R	SAS	Small angle scattering instrument
7H2R	MARX	MARX spectrometer
	SAD	Guide tube diffractometer for small angle diffraction
7H2L	TAS	Triple axis spectrometer
7H4R	PANDA	PANDA powder diffractometer

## The Mk VI Diffractometers

These two instruments are designed primarily for single crystal studies and have been robustly constructed to accept a wide range of attachments such as furnaces, cryostats and electromagnets. The basic instrument comprises an  $\Omega/2\theta$  assembly to which additional equipment is added as required. Control of the diffractometers is either manual or by a TANDON PC

### Channel 1

A two-circle attachment with  $\phi$  and  $\chi$  movements has been added to the basic unit thus converting it to a conventional four-circle diffractometer. A furnace capable of 800°C and a cryostat operating in the range 10 K to 300 K can be mounted about the  $\phi$ -axis allowing the collection of three-dimensional data at both high or low temperatures. At present, a fixed-wavelength of 1.183 Å at the sample is obtained by reflection from the (331) planes of a Cu monochromator.

This diffractometer is used primarily for structure determinations of single-crystal materials and studies of phase-transition phenomena with particular emphasis on hydrogen-bonding problems.

### Channel 2

An alternative carrier for the neutron detector shield has been added to the basic unit which permits the detector to be elevated 35° and depressed -10° from the horizontal plane, thus allowing partial three-dimensional data to be collected when using furnaces or cryostats and minimise the number of sample reorientations needed. The  $\omega$  shaft will accommodate a two-circle attachment, cryostats with arcs, furnaces and electromagnets up to a loading of 200 kg. The lower take-off angle of 45° implies that data collected at large  $2\theta$  values ( $\sim 120^\circ$ ) have poorer resolution or soller slits are available for the detector to help overcome this difficulty. The wavelength range available is 0.835 Å to 1.308 Å in discrete steps.

This instrument is used principally for studies of magnetic effects in single-crystal materials at high or low temperatures but recently it has been extensively used for structural studies at short wavelengths.

### Mk VI Diffractometers Instrument Details

Beam Hole	4H1, DIDO
Maximum Flux at Specimen	$7 \times 10^5 \text{ n cm}^{-2} \text{ s}^{-1}$
Beam Size at Specimen	$1.2 \times 0.9 \text{ cm}^2$
Background	40 cpm
Specimen Size commonly 2 or 3 mm cubes	

#### No. 1 Instrument

Incident Wavelength	1.181 Å
Take-off Angle from Monochromator	90°
Scattering Angles	(2θ) -4° to +110° (χ) +215° to -190° (φ) -187° to +187° (Ω) +231° to -205°

Cryostat for temperatures down to 10°K

#### No. 2 Instrument

Incident Wavelength	0.835, 0.886, 0.996, 1.085 and 1.308 Å
Take-off Angle from Monochromator	45°
Scattering Angles	(2θ) -20° to 133° (Ω) +200° to -217°

The vertical circle on No. 2 instrument has been removed and replaced by a cryostat for use down to 4.2°K. A lifting detector assembly has been fitted which is automatic and can be depressed by -10° and elevated to +35° from the horizontal plane.



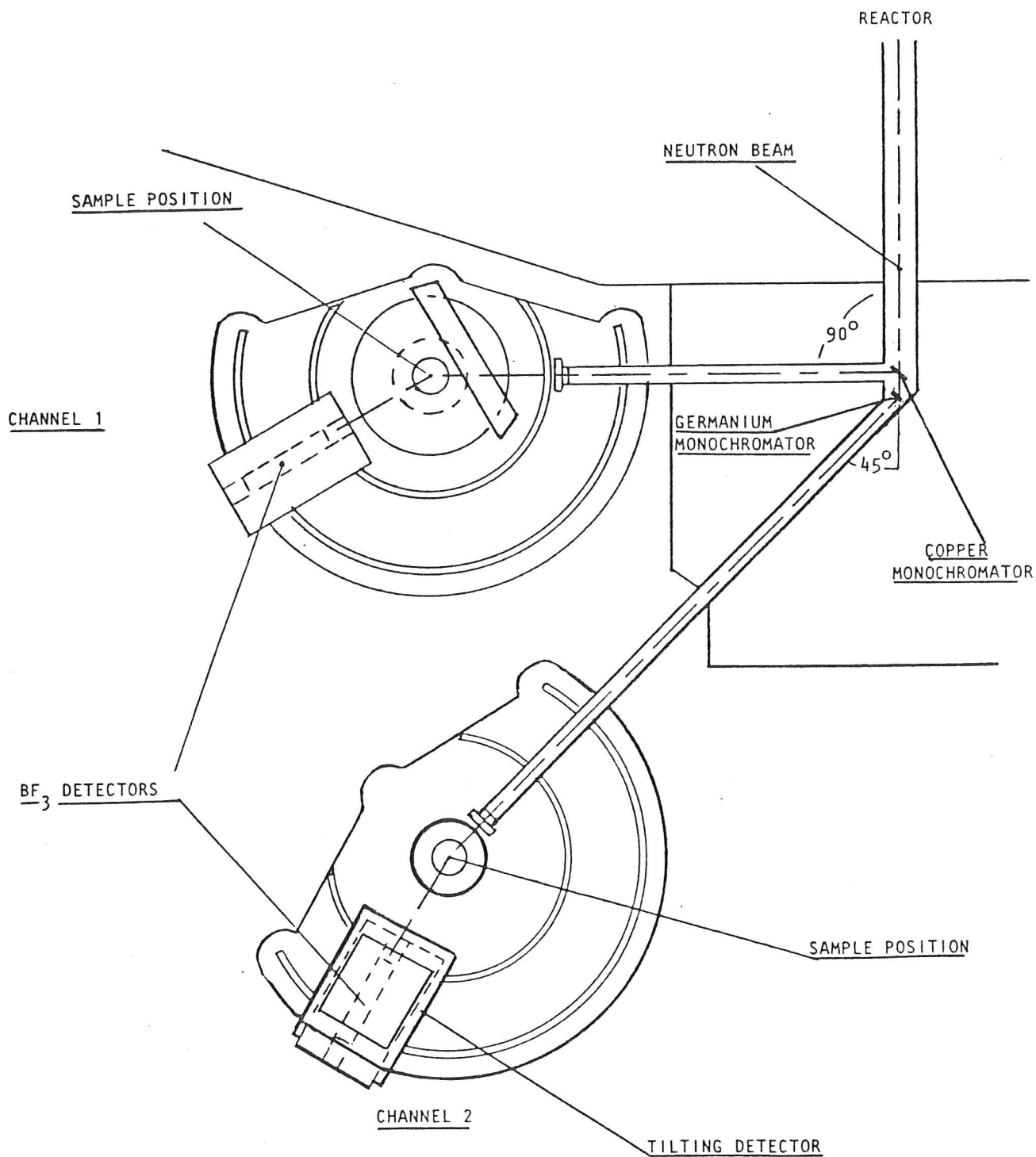


Figure 3.  
Schematic layout of mark six diffractometers



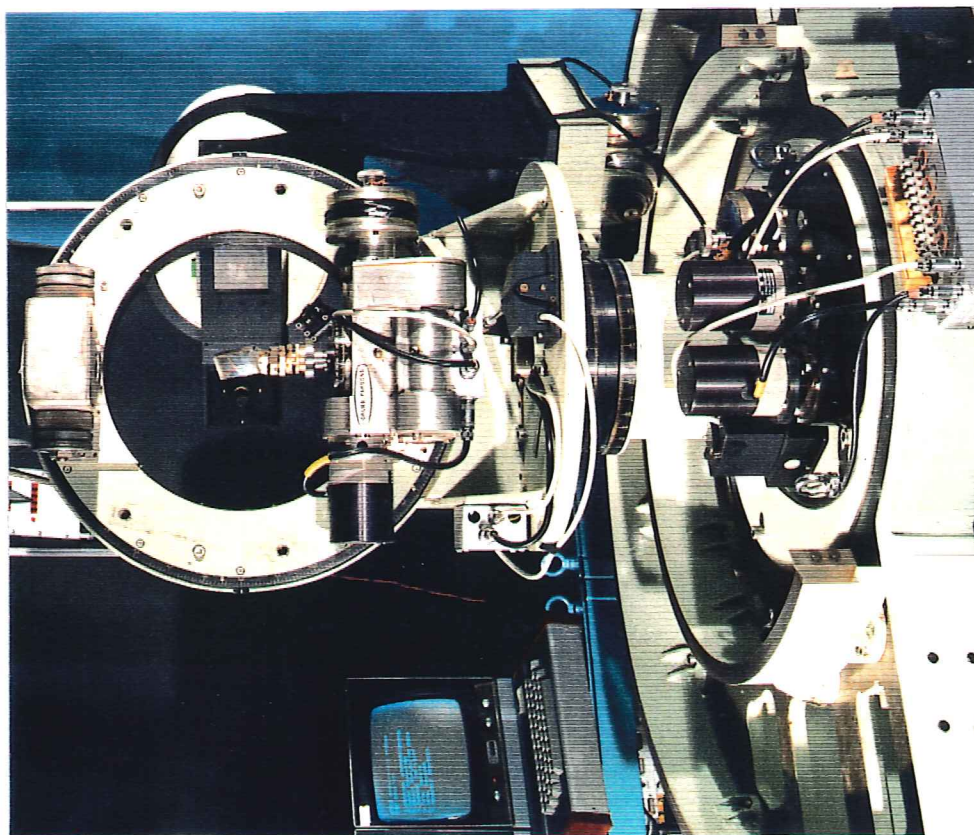


Figure 4.

Mk VI 4-circle Diffractometer  
showing sample mounted on  $\phi$  shaft.

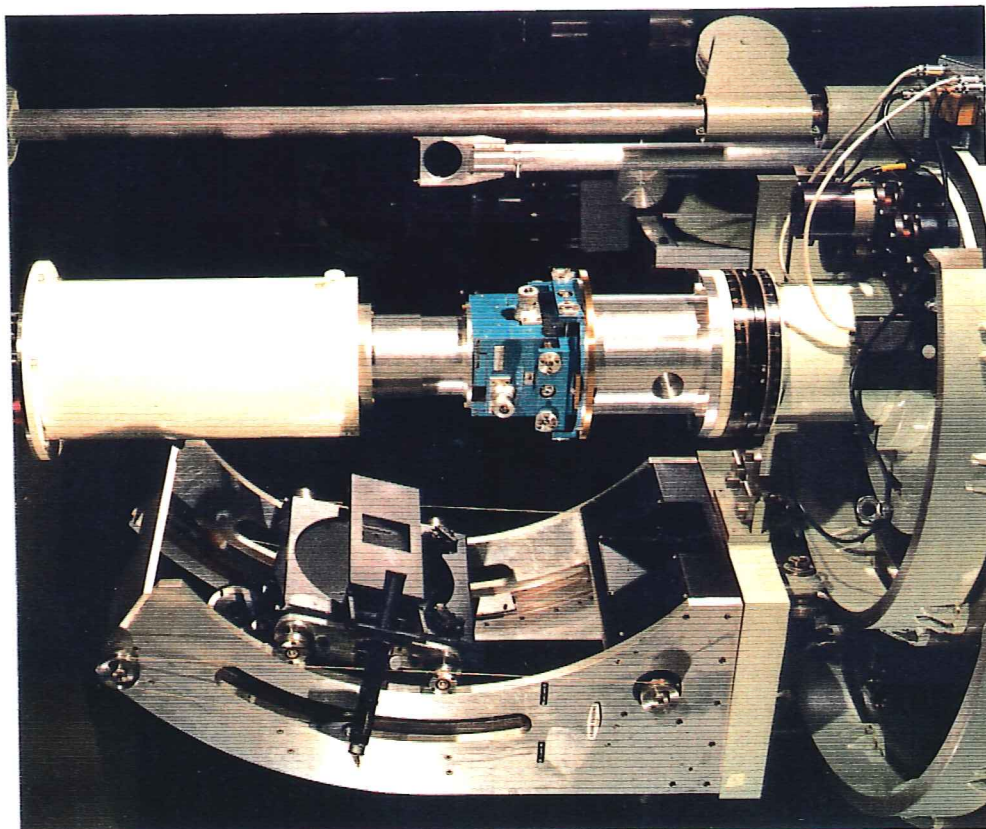


Figure 5.

Mk VI 2-circle Diffractometer with  
tilting detector and cryostat.





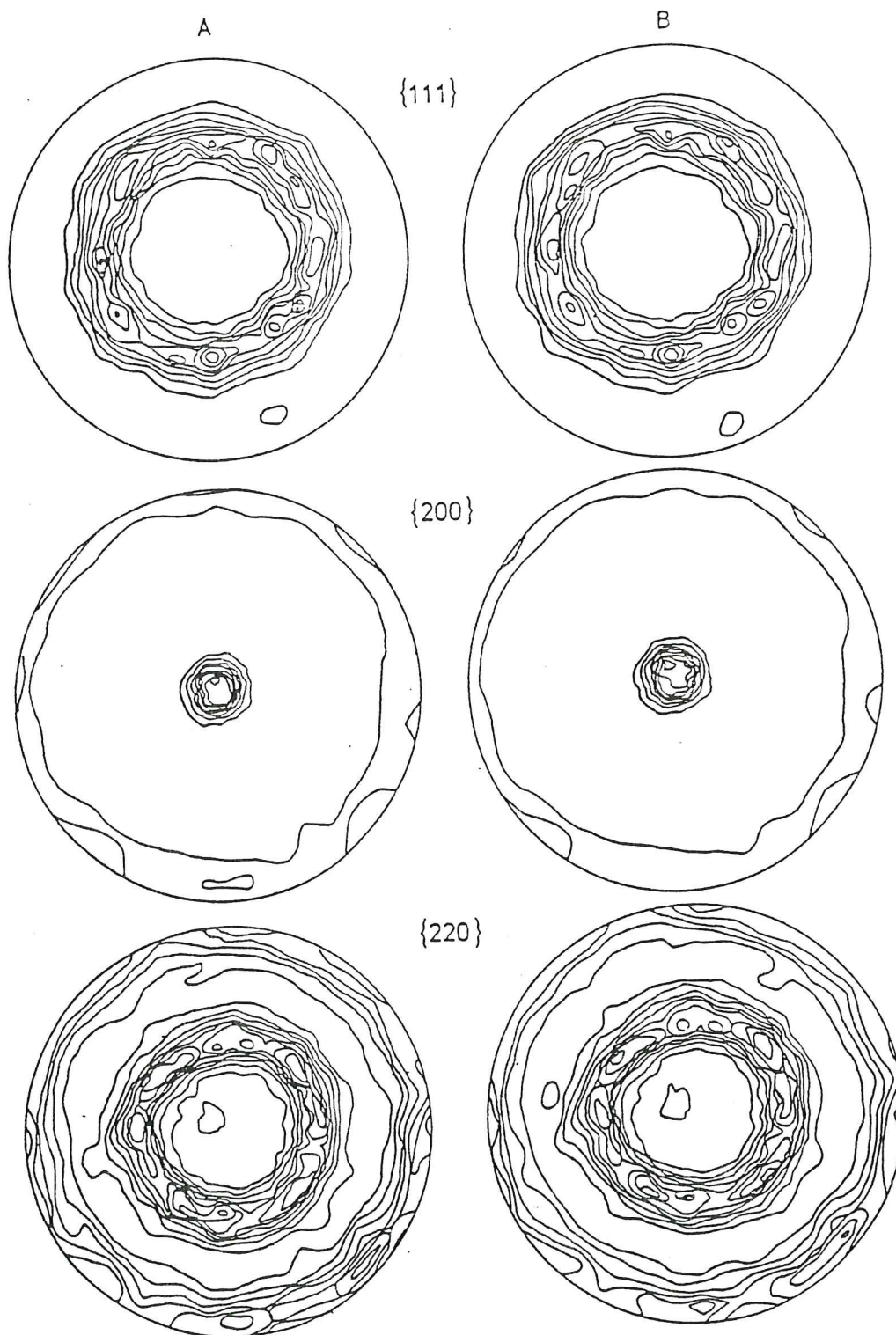


Figure 6.

Pole figures obtained on MKVI 4-circle diffractometer, showing contours of Bragg peak intensity for the reflections (111), (200) and (220) obtained from two types of scan A and B.

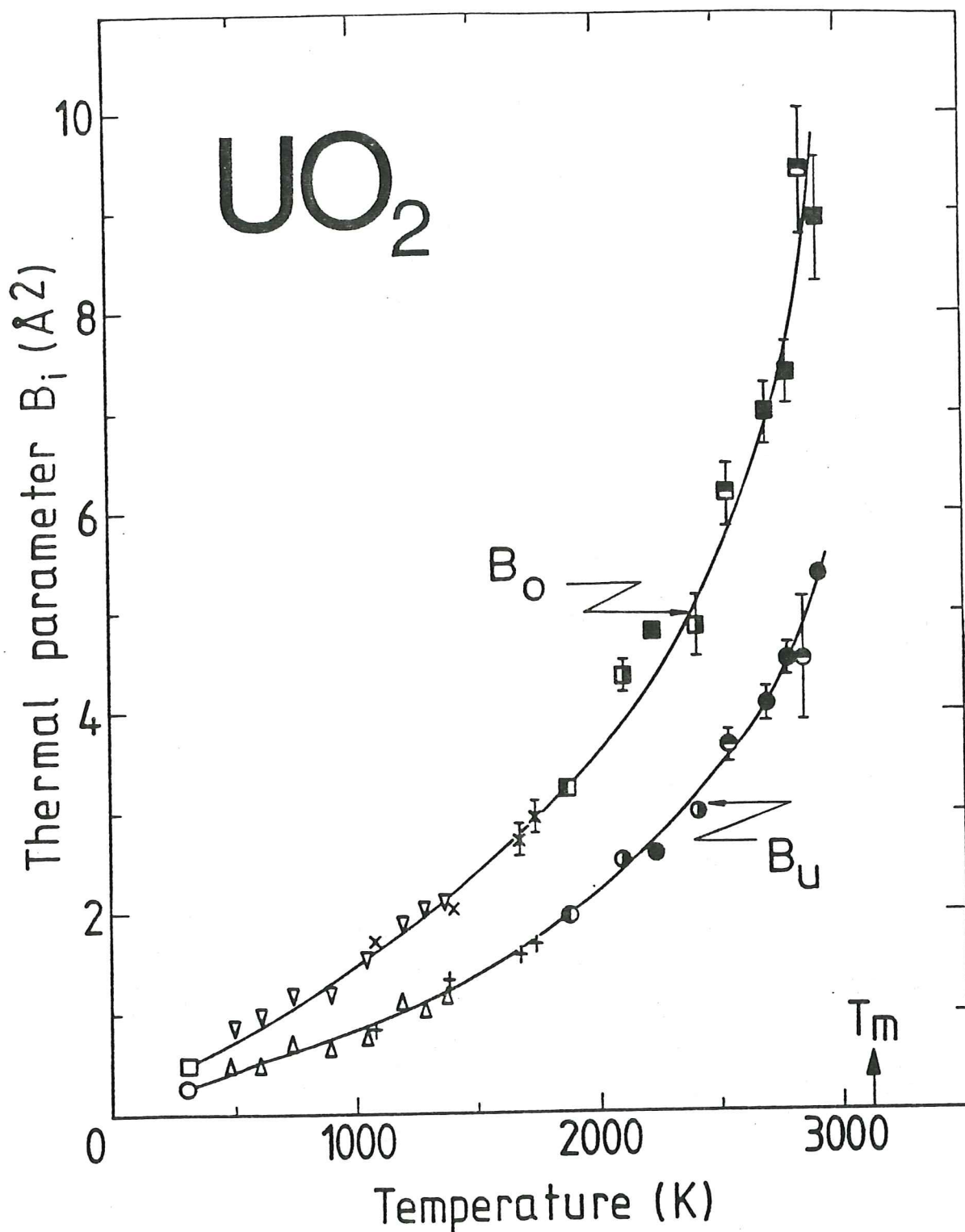


Figure 7.

Isotropic thermal parameters  $B$  for oxygen and uranium in  $\text{UO}_2$  at temperatures up to 2900K obtained using the MKVI 2-circle diffractometer.

### CURRAN Powder Diffractometer

This diffractometer is suitable for structural studies of powders, liquids and amorphous materials in the range of momentum transfer  $Q = 0.2$  to  $11.4 \text{ \AA}^{-1}$ .

The angular resolution is good ( $\sim 0.5^\circ$ ) at low values of  $2\theta$  but increases rapidly for  $2\theta > 50^\circ$ .

The background is reasonably low so the instrument is of particular value for low intensity scattering samples and experiments where it is wished to take differences between successive spectra (e.g. variable pressure and temperature runs).

There is independent  $2\theta$  and  $\omega$ -movement to facilitate the use of flat or cylindrical samples and the whole range of Harwell's cryostats, furnaces and magnets can be accommodated. There is an extract duct for potentially noxious samples.

The instrument is fully automated in operation, control and data acquisition is by an INTEL 8080 microprocessor.

# CURRAN Instrument Details

Monochromator	Ge
Take-off Angle	47.5°
Wavelength	0.90, 1.08, 1.37, 2.63 Å
Maximum Beam Size	42 × 34 mm <sup>2</sup>
Usual Sample Size	10 mm $\phi$ × 40 mm
Flux at Sample	2 × 10 <sup>6</sup> ncm <sup>-2</sup> s <sup>-1</sup> (Max)
Resolution	0.55° at 15° 0.45° at 30° 0.85° at 60° 1.55° at 80°
Angular Range	-10° to 110°
Minimum Useful Angle	~ 5°
Minimum Step Length	0.01°
Background (No Specimen)	10 cpm (2 $\theta$ =40° to 100°) 20 cpm (2 $\theta$ =5° to 40°)
Detector System	5 × 50 mm $\phi$ BF <sub>3</sub> , 10° apart Ceramic End Window
Q-Range (Å <sup>-1</sup> )	0.6 to 11.4 (0.9 Å) 0.2 to 4.8 (2.63 Å)