CLRC

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# The IRIS User-Guide

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## Preface

This is the first version of the IRIS User-Guide. IRIS is continually evolving and improving and so some of the information contained within this manual will become out of date quite quickly. The basics behind the operation of IRIS, however, should remain essentially constant for the foreseeable future. Updated manuals will be produced when appropriate although it should always be remembered that the most up-to-date sources of information concerning IRIS are the instrument scientist and the local contacts for the experiments. It would be appreciated, however, if this user-guide were to be the first point of call.

# Contents

# 1. Introduction

## 1.1 Overview

This user-guide contains some of the information necessary to conduct a neutron scattering experiment on IRIS. In order to make it as brief as possible other manuals/reports are referred to for specific details. Copies of these other sources of information are available in the IRIS Control Room (ICR). The designated local contact is also available for assistance and discussion regarding the precise details of the experiment.

The first section deals with the underlying principles governing the use of IRIS as a high resolution spectrometer and high-resolution long-wavelength diffractometer. In section 2, 'Performing an experiment on IRIS', the information is arranged so that it should be possible to perform a 'standard' IRIS experiment in a step-by-step manner. Sections 3 and 4 deal with computer control of the instrument and how to examine the data.

## 1.2 The Instrument

IRIS [1] is a high resolution inelastic neutron scattering spectrometer which also has a high-resolution, long-wavelength diffraction capability. It is an inverted geometry spectrometer which means that a range of neutron-wavelengths are incident on the sample and the scattered neutrons are energy-analysed by means of Bragg scattering from large-area crystal-analyser arrays. In common with other instruments at a pulsed neutron-source, the time-of-flight technique is used for data analysis.

The instrument is situated on the N6(A) beamline at ISIS which views the liquid hydrogen moderator (at 25 K) and so has access to a large flux of long-wavelength cold neutrons. It is convenient to consider it in two parts, the primary and secondary spectrometer. In the primary spectrometer (figure 1) the neutrons travel down to the sample position along a curved neutron guide consisting of accurately-aligned nickel-plated glass tubes which are approximately 1m-long and rectangular in cross-section. The final component of the guide system is a 2.5m-long nickel-titanium supermirror converging guide which brings the beam area down to 32 mm x 21 mm at the sample position with an increase in flux of a factor of 2.9 at 5Å. The incident flux at the sample position is nominally $5.0 \times 10^7$ n $cm^{-2}$ $s^{-1}$ (white beam at full ISIS intensity). The wavelength intensity distribution at the sample position (up to 18Å) is shown in figure 2.

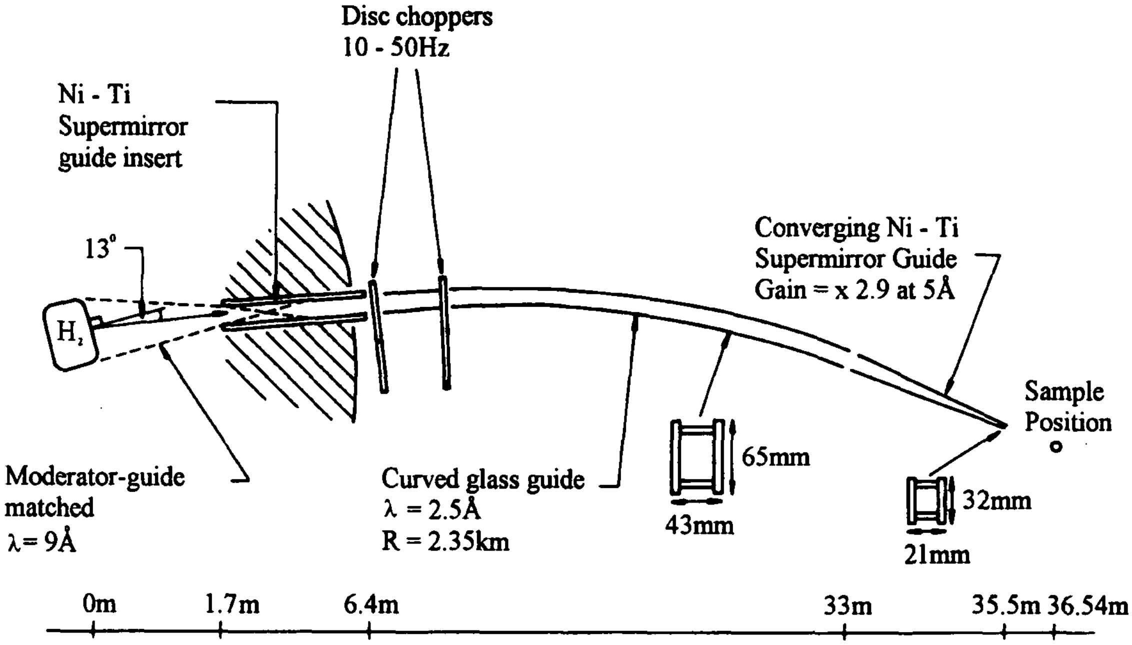



**Figure 1** The IRIS Primary spectrometer

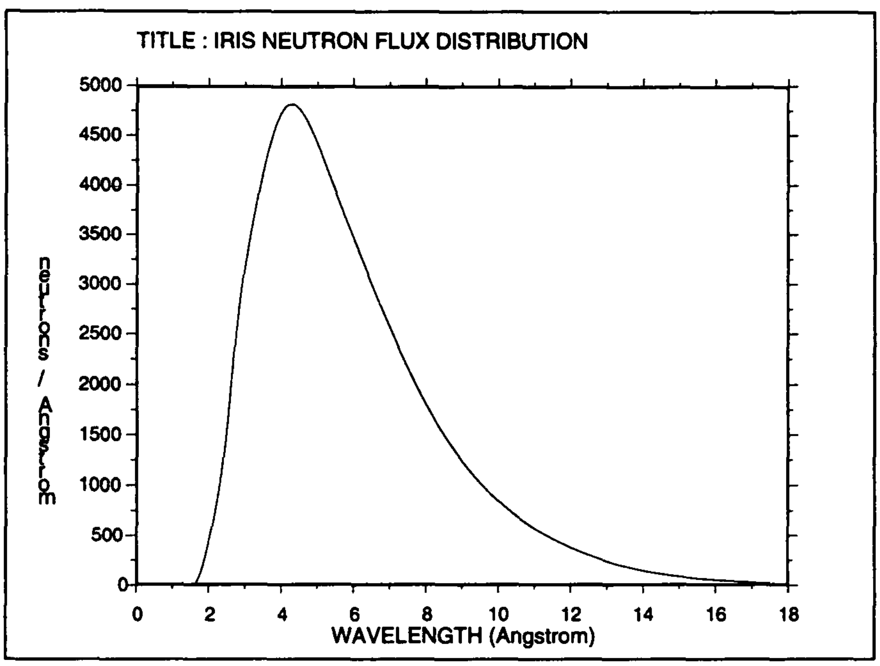



**Figure 2** Wavelength intensity distribution at sample position

The flux at longer wavelengths is still sufficient to detect bragg peaks at d-spacings of around 15Å (corresponding to ~ 30Å neutrons).

The wavelength intensity distribution in figure 2 bears little resemblance to the incident flux observed during real experiments. This is because after leaving the moderator the neutrons pass through two disc-choppers, consisting of discs of neutron-absorbing material with adjustable apertures. These are used to define the range of wavelengths within the incident beam and also to avoid the frame-overlap problem in which the faster neutrons in one pulse catch up with the much slower, long-wavelength neutrons in the preceding pulses. This mixing of pulses makes data analysis by time-of-flight very difficult. The disc-choppers can be set to operate at a number of frequencies and are synchronised to the operation of the neutron source. The size of the wavelength-bands can be changed by adjusting the operating frequency. The size of the apertures can also be adjusted to do the same thing but this can only be done manually so in practice the apertures are kept fixed to provide wavelength-bands which are 2Å wide when operating at 50Hz. The lower and upper limits of these wavelength bands are defined by adjusting the phase or time-delay of the opening of the aperture relative to the time, commonly referred to as "$t_0$", that the neutrons are produced at the target. This wavelength-band selection effectively defines the energy resolution and energy-transfer range (inelastic) or d-spacing range (elastic) covered during the experiment.

The secondary spectrometer consists of a 2m diameter vacuum vessel containing two crystal analyser arrays (pyrolytic graphite and mica), two 51-element ZnS scintillator detector banks and a diffraction detector bank at $2\theta=170°$ containing ten $^3He$ gas-tubes (fig. 3). There are also a number of beam monitors to determine the wavelength distribution both incident upon the sample and after the sample. The graphite analyser bank is cooled to close to liquid helium temperatures in order to reduce background from thermal diffuse scattering.

## 1.3 Basics of IRIS operation

### 1.3.1 Inelastic scattering

For inelastic scattering measurements the neutrons scattered from the sample are energy-analysed by Bragg-scattering from the arrays of single crystals. Only neutrons with the appropriate energy (as determined by the Bragg condition) are directed towards the detectors. The time-of-arrival of these neutrons (relative to $t_0$) is recorded and the energy exchanges which have taken place within the sample can then be calculated (refer to figure 4).

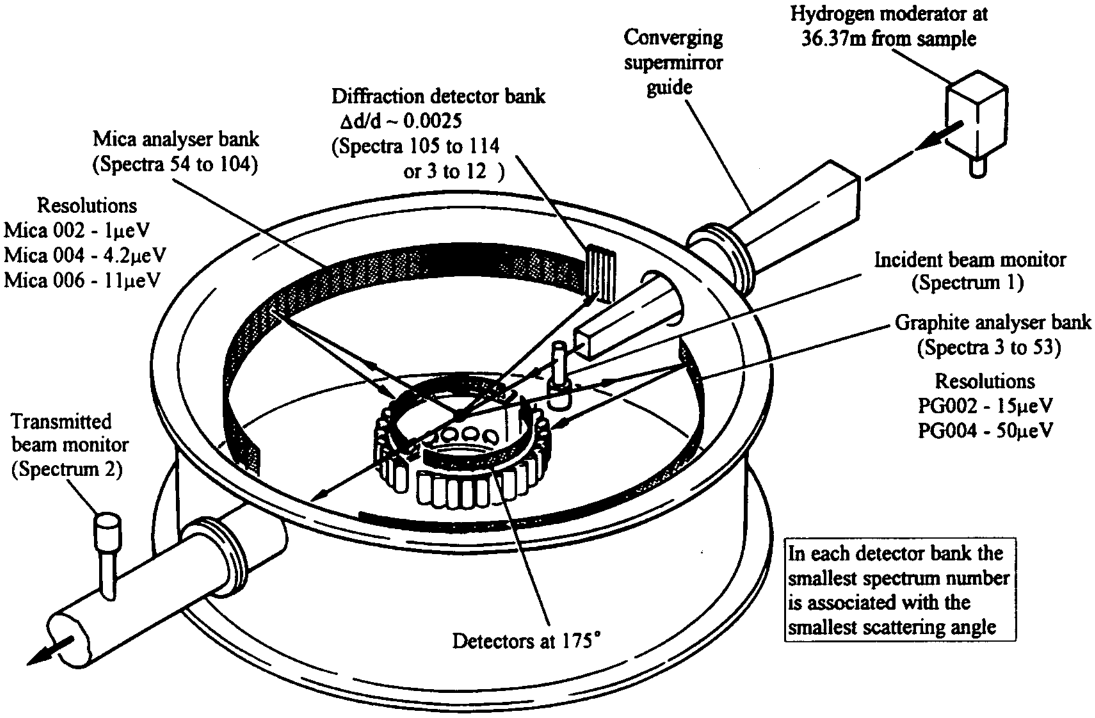



**Figure 3** The IRIS secondary spectrometer

The neutrons incident on the sample, S, coming from the moderator, M, have a range of energies and so the time-of-flight, $t_1$, along the incident flight path, $L_1$, is variable. However, of the neutrons scattered at an angle $\phi$, for example, only those with a final energy $E_2$ which satisfies the conditions expressed in equations 1-4 (over the page) can reach the detectors, D.

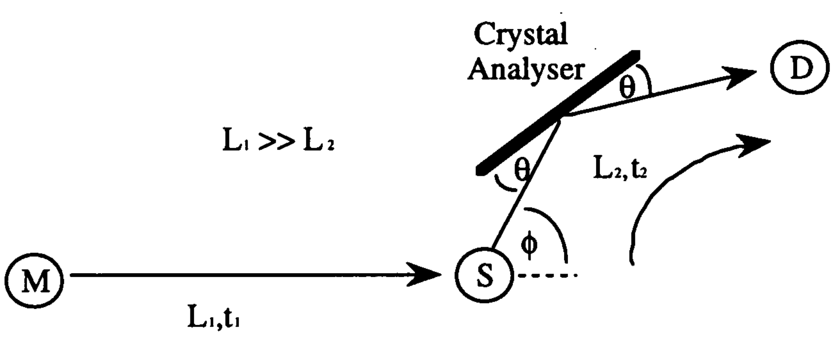



**Figure 4** An indirect-geometry inelastic neutron scattering spectrometer.

$$p = m_n v = \frac{h}{\lambda} \qquad \text{(de Broglie)} \qquad (1)$$

($m_n$ is the mass of the neutron)

$$\lambda = 2d\sin\theta \qquad \text{(Bragg)} \qquad (2)$$

$$E_2 = \frac{1}{2}m_n\left(\frac{L_2}{t_2}\right)^2 = \frac{1}{2}m_n v^2 = \frac{p^2}{2m_n} = \frac{1}{2m_n}\left(\frac{h}{\lambda_a}\right)^2 = \frac{1}{2m_n}\left(\frac{h}{2d_a\sin\theta}\right)^2 \qquad (3)$$

where $d_a$ is the analyser d-spacing.

Therefore the time-of-flight of the neutrons, $t_2$, which are able to traverse the secondary flight-path, $L_2$, is fixed and given by:

$$t_2 = \frac{2m_n L_2 d_a \sin\theta}{h} \qquad (4)$$

Thus by measuring the total time-of-flight, t ($=t_1+t_2$), and knowing $t_2$, $L_1$ and $L_2$ the energy exchange within the sample can be calculated from:

$$\Delta E = E_1 - E_2 = \frac{1}{2}m_n\left[\left(\frac{L_1}{(t-t_2)}\right)^2 - \left(\frac{L_2}{t_2}\right)^2\right] \qquad (5)$$

1.3.2. Diffraction

The diffraction detector bank at close to backscattering is used either to measure crystallographic parameters simultaneously with the dynamical information or for structure determination purposes in purely diffraction experiments. The neutrons scattered from the sample reach the diffraction detectors directly but time-of-flight analysis is still used to calculate the d-spacing of the observed reflections. In this case the scattering geometry is simplified (figure 5) with the scattering angle 2θ replacing the scattering angle ϕ in the previous figure. The calculation of d-spacing values from the time-of-flight measurements is also more straightforward.

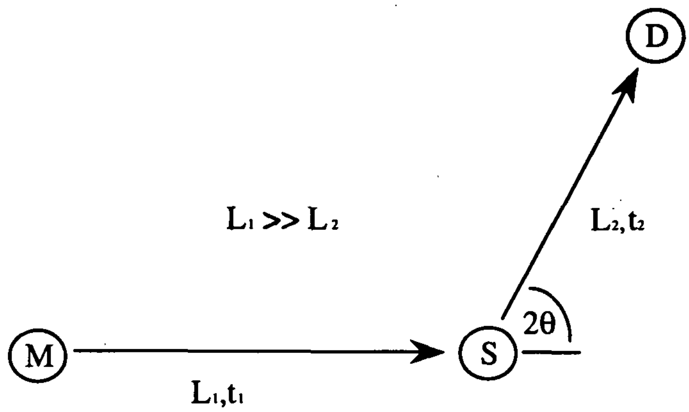



**Figure 5** A simple diffractometer

From equations 1 and 2:

$$m_n\left(\frac{L}{t}\right)=\frac{h}{\lambda}=\frac{h}{2d_s sin\theta} \tag{6}$$

where L is the total flight-path, $L_1 + L_2$, t is the total flight-time, $t_1 + t_2$, and $d_s$ refers to the set of d-spacings for the sample which are therefore given by:

$$d_s=\frac{ht}{2m_n L sin\theta} \tag{7}$$

# 2. Performing an experiment on IRIS

## 2.1 What to do before arriving at IRIS

There are a number of administrative procedures to be followed before arriving at the spectrometer. Missing out on any of these **will** delay the start of the experiment.

### 2.1.1 The ULS, MCR, film badges, swipe cards and safety video

Upon arriving at ISIS users should go to the University Liaison Secretariat (ULS) in R3 where arrival should be registered/recorded. First-time users should be given an information-pack about ISIS and all aspects of safety at ISIS. They will also be required to watch the ISIS Safety Video. They will then be directed to the ISIS Main Control room (MCR) or perhaps the office of the local contact for the experiment.

Outside office hours the MCR will hand out safety information but at the earliest available opportunity arrival should be registered at the ULS.

Before entering building R55 a radiation badge and a 'swipe-card' for the security systems is required. They are obtained at the MCR.

### 2.1.2 Sample safety assessment

All users complete a "Sample Record Sheet" as part of their application for beamtime ,the information being used to carry out a sample safety assessment. This will give comments from the ISIS Safety Section concerning possible chemical or radiological hazards associated with the sample/experiment and any recommendations concerning sample handling, etc. **These must be followed**.

Before beginning their experiment the user should collect their sample safety assessment sheet from the filing cabinet in the Data Assessment Centre (DAC) ( building R55 ) and display it in the pocket attached to the sample enclosure area for the duration of the experiment. The user should have viewed the safety video and also read the safety handouts given to them when they arrived.

## 2.2 Selecting sample cans and scattering geometry

An important decision to make is the selection of the optimal scattering geometry and sample can for the experiment. In many cases the selection of can is determined by the form of the sample and/or the sample environment. If this is not the case then the following will help in deciding upon the type of can and scattering geometry.

### 2.2.1 Flat plate cans

In these cans the sample area is nominally 40 by 40 mm and there are a number of different sample thickness available. The selection of sample thickness is determined by the scattering strength of the sample - a 10-15% scatterer is the ideal (multiple scattering is, in general, not a problem at this level). The scattering strength of the sample can be roughly calculated using the following equation :

$$I = I_0 \exp(-n\sigma t)$$

i.e.

$$t = -\frac{1}{n\sigma}\ln\left(\frac{I}{I_0}\right)$$

where $I_0$ is the incident intensity, $I$ is the transmitted intensity, n is the number of scattering atoms per unit volume, $\sigma$ is the 'average' scattering cross-section for the atoms in the sample and t is the thickness of the sample. For example, for a transmission of 85% (scattering of 15% ignoring absorption processes) then:

$$t = -\frac{1}{n\sigma}\ln(0.85)$$

More specifically, for polyatomic samples, $n\sigma=(n_1\sigma_1+n_2\sigma_2+n_3\sigma_3+...)$ but in many cases all atoms apart from hydrogen can be ignored because it has by far the largest incoherent scattering cross-section.

These cans can be sealed with indium or 'o'-rings and can be used for liquids as well as powders. The big advantage of using these cans is that the design specifically incorporates holes for cartridge heaters and temperature sensors which enables quick and very fine temperature changes and control. However, the heaters and sensors have to be shielded using cadmium sheet which means that scattering in the plane of the sample will be greatly reduced and so sample orientation is important. The sample must be aligned appropriately for your experiment. Usually this means orienting the sample at ±45° relative to the incident neutron beam (straight-through is 0° and exact backscattering is 180° - the angles on the graphite side of the instrument are defined as being positive and the angles on the mica side are negative). The decision regarding the sample orientation depends specifically upon the Q-range and energy-resolution required for the experiment. Cases to consider are:

a) High-Q: If high-Q values are required for a particular resolution (e.g. tunnelling experiments) then reflection geometry is best (e.g. plane of sample at +45° which means that the 'blind spot' occurs at low angles). If the graphite analyser is being viewed with this scattering geometry then this also gives access simultaneously to low-Q on the mica side of the instrument as long as the back of the sample is not shielded with cadmium. This is possible because both the graphite 002 and mica 006 reflections make use of the same wavelength band. If both Q-ranges are not required then shielding the back of the sample with cadmium will reduce background scattering from the sample environment equipment.

b) Low-Q: If low-Q values are required then transmission geometry should be employed. A sample orientation of +135° is ideal for some magnetic scattering experiments in which the graphite 004 reflection is used (for its larger energy transfer range) but optimising the scattering on the lowest possible Q-values where the magnetic scattering is strongest. This scattering geometry will also give a better diffraction pattern because of the position of the diffraction detector on the mica side of the instrument. It should also be noted that spurious signals due to bragg scattering will be reduced at low angles.

c) Both the above sample orientations (with negative instead of positive angles) will work for the mica reflections (002,004,006) but only the mica 006 reflection will enable the simultaneous use of the graphite analyser.

2.2.2 Annular/cylindrical cans

The external diameter of these cans is 20 mm and the internal diameter is 19.5 mm which gives the maximum size of cylindrical sample that can be accommodated. The height of the cells is nominally 5 cm. They come with hollow cylindrical inserts which in combination with the main body of the cell produce an annular cross-section (as viewed from above) for the sample with thickness ranging from 0.5 to 2 mm. The advantage of this geometry is that there are no edge effects as in the case of the flat plate cans and the potential for multiple scattering problems is reduced. The can orientation is not important unless heaters and temperature sensors have been attached. Without heaters/sensors there are no 'blind spots' and so if "Q-variation" is the most important information to be extracted from the experiment then this is the scattering geometry to go for.

## 2.3 Loading a sample into the neutron beam.

Most experiments on IRIS make use of a 100mm-bore "Orange" cryostat. There should be an operations card detailing it's usage in the pocket attached to the cryostat's trolley. If one is not available, inform the local contact who will obtain a replacement and/or go through the operation of the cryostat and sample loading procedure. The local contact will also provide the necessary advice and assistance on how to load samples if a different sample environment kit is to be used.

## 2.4 Opening the beam shutter

Before the beam shutter can be opened to allow neutrons onto the sample the beam interlocks have to be set. The interlock system consists of two parts; that associated with the control of the main shutter which affects both the IRIS and OSIRIS beamlines (N6A and N6B) and that associated with the IRIS intermediate shutter. During a running period there should only be a few occasions when it is necessary to open/close the main shutter and this should **ONLY** be done under the supervision of the instrument scientist or local contact. The intermediate shutter control system can be operated by visitors alone after suitable instruction. It consists of a set of keys with corresponding locks and a button for open and close. There is a master key (N6A-M) and three "A"-keys labelled N6A-A. The shutter cannot be opened unless all four of these keys are in their appropriate locks.

Inserting and turning (clockwise) all the A-keys in their locks in the A-key box will enable the removal of the master key which can then be inserted into the lock in the master key box. Once the master key is in and turned the shutter can be opened by pressing the open button of the shutter control box. The local contact will point out the location of these boxes and demonstrate how the interlock system operates.

Once the open button is pressed the master key is locked into its box and cannot be removed until the shutter is closed. In principle this means that all active areas on the beamline are inaccessible whilst the shutter is open. At the time of going to press access to the area underneath the instrument (which is necessary for some instrument operations) is only available after closing the main shutter and so can only be done under the supervision of the local contact or instrument scientist.

Gaining access to an interlocked area (the sample environment area for example, requires that the shutter be closed before the necessary keys can be made available for entry. The procedure is essentially the reverse of the above. The shutter is closed, the master key is removed and put into it's lock in the A-key box. This releases the A-keys for access to interlocked areas.

## 2.5 IRIS Computing overview

A 333 MHz DEC Alpha Workstation is used for all aspects of instrument control and data analysis. It is commonly referred to as the IRIS FEM (Front End Minicomputer). The workstation makes use of the DEC OPENVMS operating system. Details of the older, but essentially similar, VAX/VMS operating system can be found in the PUNCH manual [2]- a copy of which is available in the ICR. Alternatively, ISIS computer support group (on extensions 5414 or 3029) can answer questions about the operation of the workstation.

As well as the ALPHA workstation there is an older VAX 3600 and a PC available in the ICR. All can be used to access the FEM and other areas of the network.

The ALPHA workstation is set up to use the DECWINDOWS windows management system. This has the advantage of enabling the use of automatic start-up for the standard windows used for instrument control and data analysis. If there are no windows present on the screen then click on the OPTIONS button and then the SESSION button. Next select the DECWINDOWS session option before entering the username IRIS and the current IRIS password (available from the local contact). This will ensure that upon start-up the necessary windows are automatically generated.

The windows that should be started are: IRIS Control and Dashboard. The IRIS Control window is where all the instrument control commands should be typed. The Dashboard window provides information about the current instrument status (see section 3.1.4).

Other windows which can be generated from the IRIS menu on the session manger window are: IGIS, ZEUS, GENIE and OPENGENIE. IGIS is a graphical interface for the IRIS

Data Analysis package IDA [3], ZEUS is an interactive analysis and display package, GENIE is a display package common to all instrument at ISIS and OPENGENIE is it's replacement.

## 2.6 Selecting suitable instrument settings for the experiment

IRIS can be easily configured to match the physical problem that is under investigation. In essence it is just a matter of selecting an appropriate resolution and energy-transfer-range or, in the case of diffraction, appropriate d-spacing ranges. For inelastic scattering different resolutions are associated with the different analyser reflections available. Selection of a particular analyser reflection (and hence resolution) and energy-transfer-range is achieved by defining: the frequency and phases (time-delay settings relative to $t_0$) of the two disc-choppers, and the time-channel-boundaries (TCB's) for data acquisition. The procedure is the same for selecting a particular d-spacing range. The selected configuration is implemented by issuing commands in the IRIS Control window on the FEM.

The current standard settings of the instrument can be found in Appendix I and the recommended chopper phases are available in the ICR. Many of the standard settings are available by modifying standard files with the extension .CRPT (see section 3.1.2) and then typing single word commands in the IRIS Control window. These commands are also shown in Appendix I along with the name of the appropriate .CRPT files which need to be edited beforehand. For non-standard settings a program called IRIS_SETTINGS is available. This program will predict the appropriate time channel boundaries and chopper phases for the required energy-transfer and d-spacing ranges. However, in many cases the nature of the sample or the physical problem being investigated will mean that these settings are not appropriate because of the presence of spurious peaks or overlap between scattering from different analyser reflections. Advice must be sought from the local contact or instrument scientist.

## 2.7 Chopper control

Having decided upon an appropriate configuration the first thing to do is to set the chopper frequencies and phases. There are two disc choppers at approximately 6.3m and 10m from the source. They are referred to as the six-metre and ten-metre choppers respectively.

2.7.1 Changing the chopper frequency

The IRIS disc-choppers operate at the following frequencies: 50Hz, 25Hz, 16.7Hz, 12.5Hz and 10Hz. To change the frequency the following command is used:

FREQ'n' 'm'

where 'n' is either 6 or 10 and 'm' is the required frequency. For example the command:

FREQ6 25

will set the frequency of the 6m chopper to 25 Hz.

Because the ISIS timing signal from ISIS comes into the 6m chopper electronics crate into which the 10m chopper is linked, **it is important that the frequency of the 6m chopper is changed first** and some time allowed (one minute will suffice) before changing the frequency of the 10m chopper.

2.7.2 Changing the chopper phases

After the required frequencies have been attained, the phases can then be set.

PHASE6 1000

will set the phase of the 6m chopper to 1000μs.

The frequencies and phases of the two choppers can be adjusted manually if there is a problem with the computer control. This should only be done with the consent of and under instruction from the local contact or instrument scientist.

## 2.8 Data collection

### 2.8.1 CHANGE

Typing CHANGE <CR> in the IRIS Control window will enter the DEFT screen editor and allow parameters within the Current Run Parameter Table (CRPT) such as the monitor range, time-channel-boundaries (TCB's) and the title of the experiment to be modified. Key number 7 on the right-hand keypad of the keyboard will page through the screens and by using the up and down cursor arrows different data fields on each page can be accessed. Basically all that is required is to type in an appropriate title, enter the correct TCB's (in micro-seconds), enter the correct monitor range (in micro-seconds) and if going from an inelastic set-up to a diffraction set-up (or vice-versa) then change the spectra table (SPECTRA.DAT for inelastic experiments and DIFFSPECTRA.DAT for diffraction experiments). No other input is necessary although information such as type of sample can, orientation and scattering geometry can also be entered. To exit from the editor press the 'PF1' key on the right hand keypad followed by 'E' for Exit. A successful edit will produce the following responses: "values written to INST.UPD" and "all parameters updated successfully".

### 2.8.2 BEGIN

To start the run type BEGIN (again in the IRIS control window). After a few seconds the dashboard should indicate that IRIS is RUNNING and the total number of micro-amps and the monitor counts will begin to increment.

### 2.8.3 Data inspection

To inspect the data as it is being accumulated the programs GENIE and ZEUS which are discussed in section 3.2.1 can be used. These programs will enable a decision as to when it is appropriate to end the run.

### 2.8.4 END and end of experiment

Once the data collected is of sufficient quality then typing END will stop the run and store the data. The data is automatically archived after a few minutes onto an optical disk storage system.

At the end of the experiment (which may consist of a number of runs under different conditions and using different instrument configurations) each sample (in its can) should be monitored for induced radioactivity and then dealt with using the recommended procedure for dealing with active samples (handout on health physics in ICR). Assistance in this task can be obtained from the ISIS Health Physics Office (6696) or the ISIS Main Control Room (6789).

If the sample is not active it should be removed from its can, the can cleaned ready for the next users and the sample dealt with as according to the sample safety assessment (stored at ISIS, removed from ISIS or disposed of by ISIS staff).

If removal of the sample from ISIS is required and it is not possible to do this immediately because of the induced activity, arrangements should be made with the local contact to remove it at the earliest available opportunity. All the samples stored in the Active Sample cupboard should be logged in (on storage) and out (upon removal) in the logbook located on the inside of the cupboard door. It is not guaranteed that samples will remain stored at ISIS indefinitely.

It may be possible, with the assistance of Radiation Protection (6696), to package an active sample in such a way as to make its removal from ISIS safe.

Before leaving, all film badges and swipe cards should be returned to the MCR.

# 3. IRIS computing

## 3.1 Instrument Control

### 3.1.1 The Data Acquisition Electronics

During the course of a run, data is accumulated in the Data Acquisition Electronics (DAE) in a number of spectra, each corresponding to a particular detector. Each of these spectra contains a histogram of neutron counts versus time-of-flight. At the end of the run the contents of the DAE are automatically copied to a file on the FEM (Front End Minicomputer) called IRSnnnnn.RAW, where 'nnnnn' is a five figure run number which is incremented automatically at the end of each run. Shortly after creation, this RAW file is also archived onto optical disk. The DAE has four possible states:

| | |
|---|---|
| SETUP | Data is not currently being collected. The instrument parameters may be changed if required before starting a new run |
| RUNNING | Data is currently being collected and stored in the DAE |
| PAUSED | Data collection is temporarily suspended by the user |
| WAITING | Data collection is temporarily suspended by the FEM. This may occur, for example, when a cryostat temperature is outside the defined temperature limits |

The current DAE mode and run status are displayed on the dashboard.

### 3.1.2 The CRPT

The Current Run Parameter Table (CRPT) contains additional information on the current run, and is copied along with the contents of the DAE, to the RAW file on the FEM at the end of the run. It contains information such as the title of the experiment/run, users' names, etc. plus details of the instrument configuration and settings (the TCB's, the detector used as the monitor spectrum, etc.).

### 3.1.3 The ICP

Data collection on ISIS instruments is controlled by the Instrument Control Program (ICP). This program is used to start and stop data collection, but also allows data collection to be suspended temporarily to allow, for example, entry into an active area. Data collection can also be suspended automatically if the CAMAC-based sample environment control system indicates that, for example, the temperature has gone outside of pre-defined limits. The available ICP commands which are most widely used are:

| Command | Effect |
|---|---|
| CHANGE | Enables the contents of the CRPT to be modified |
| BEGIN | Clears DAE memory,<br>Sets parameters in DAE to those specified by the CRPT<br>Instructs DAE to start data collection<br>Sets DAE state to RUNNING (indicated on the Dashboard) |
| PAUSE | Suspends data collection by the DAE<br>Sets DAE state to PAUSED |
| RESUME | Resumes data collection by the DAE<br>Sets DAE state to RUNNING |
| UPDATE | Suspends data collection by the DAE<br>Copies contents of DAE to the CRPT<br>Restarts data collection by the DAE |
| STORE | Suspends data collection by the DAE<br>Copies contents of the CRPT to the file IRSnnnnn.SAV<br>Restarts data collection by the DAE |
| ABORT | Stops data collection by DAE<br>Does NOT store data<br>Sets DAE state to SETUP |

END — Stops data collection by DAE

Copies contents of DAE memory and CRPT to file

IRSnnnnn.RAW

Increments the run number 'nnnnn'

Sets DAE state to SETUP

The CHANGE command requires some further explanation as it involves the use of the DEFT editor (section 5.1.4 of the PUNCH manual). After typing CHANGE and thus entering DEFT then button number 7 on the right-hand keypad will page through the screens and within each screen. To move from one field to another (for data entry) the 'up' and 'down' cursor arrow keys should be used. When the file prompts with 'toggle data type' the '.' key on the right hand keypad should be pressed until the field displays the required option. All other fields are altered by typing the appropriate numbers or characters into the field, the 'left' and 'right' cursor arrow keys, the 'delete' key and space bar allow corrections to be made. To exit from the editor and overwrite the CRPT with the new values the user should press the 'F1' or 'PF1' key on the right hand keypad, then press the key 'E' for Exit. If you wish to quit and leave the editor without overwriting the CRPT then press 'Q' for Quit.

During the course of an experiment some simple alterations to the CRPT can be made without using the DEFT editor. These can be typed at the keyboard or given from a command file, regardless of the DAE state. For example:

CHANGE TITLE """4-Methyl Pyridine at 10 kbar and 4.2K""" <CR>

will alter the title of the current experiment. The treble quotes ensure that the title is reproduced literally with upper and lower case characters, spaces etc.

The ABORT command does not store the accumulated data and so should only be used if it is certain that the data is not needed. If ABORT is issued accidentally it is possible to recover the data using the program RECOVER, but only if a BEGIN command is not issued (this clears the DAE memory). Within the IRIS CONTROL window (or wherever the BEGIN and ABORT commands were issued) type at the prompt:

RUN SYS$PUBLIC:RECOVER

### 3.1.4 The Dashboard

The IRIS instrument dashboard is contained in a separate window on the FEM. It displays information concerning the current run. At the top of the dashboard the current DAE state (RUNNING, SETUP, etc.) and the run number are shown. The remaining information on the dashboard includes the user, sample, run time, frame (proton pulse) count, present and accumulated proton beam current, the incident beam monitor counts and sample environment parameters being monitored by CAMAC.

### 3.1.5 SECS, CAMAC and Eurotherms

A complete description of the Sample Environment Control System (SECS) can be found in the PUNCH manual (section 5.2). The commands which the user will find most useful are those involved in controlling temperature. The temperatures of the sample or sample environment equipment can be set as well as logged from any computer terminals logged onto the IRIS FEM. In addition, data collection can be temporarily suspended when a specified temperature reading goes outside of a specified range.

Basically there are three aspects to the temperature control system. The FEM (for issuing the commands), the CAMAC unit (hardware/software interface) and the Eurotherm temperature controllers. The temperature controllers measure the millivolt output from resistance thermometers (Rh/Fe or Pt) or thermocouples (usually type-K) and control the temperature at a specified setpoint using a 3-term control algorithm (proportional band, integral time and derivative time - commonly referred to as PID control).

The conversion from millivolts to K or °C is done using tables held on the mainframe (each Rh/Fe sensor for example is calibrated at a number of points and has its own conversion table and identification number). The units depend upon the sample environment equipment in use but would normally be K for a cryostat and °C for a furnace. The dashboard usually displays both the millivolt readings and the converted values. TEMP and TEMP1 are the two software control blocks in the SECS which correspond to the two EUROTHERM temperature controllers.

### 3.1.6 Temperature control

Following are a few examples of the more useful commands in the SECS relating to the control of temperature:

CSET TEMP/LOG or CSET TEMP1/LOG

These commands will cause the readings observed in the temperature control blocks, TEMP and TEMP1, to be logged. Each time an IRIS run is ended the a temperature log file is closed and a new one opened. These files are called IRSnnnnn.LOG where, as before, 'nnnnn' is the run number. The .LOG files are stored on the FEM and archived to optical disk in the same fashion as the RAW and SAV files.

CSET TEMP/DEVSPEC = 5864

This command informs the SECS which calibration table should be used for the conversion from mV to Kelvin for the control block TEMP (associated with Rh/Fe sensor number 5864 - the sensor numbers are written on the side of the sensors).

CSET TEMP/DEVSPEC = -2

This command informs the control system that a type-K thermocouple is being used.

CSET TEMP/PROP = 2

This command sets the proportional band of the temperature control loop to 2% of the setpoint value.

CSET TEMP/INT = 500

This command sets the integral time to 500 seconds.

CSET TEMP/DERIV = 100

This command sets the derivative time to 100 seconds.

CSET TEMP/VALUE=15/LOLIMIT=10/HILIMIT=20/CONTROL

This command results in a setpoint value of 15 (K or °C ) being issued to the temperature controller associated with the control block TEMP. The controller will attempt to maintain a temperature of 15 (K or °C). The low and high limits are not transferred to the temperature controller but are used by the ICP to inhibit data collection because of the /CONTROL prompt. If the value of TEMP varies outside this range the ICP makes IRIS go into the WAITING state until the value returns into the range. This data collection vetoing can be disabled by issuing the command:

CSET TEMP/NOCONTROL

Information on the current status of TEMP and TEMP1 can be obtained by typing:

CSHOW TEMP or CSHOW TEMP1

The setpoint value and limits will be shown as well as an indication of whether this value is being logged and used as a control parameter (in the form T or F for true or false).

CSHOW CAMAC/OUT_OF_RANGE and CSHOW CAMAC/CONTROL

will indicate which blocks are causing data collection to be inhibited and those in use as control parameters, respectively.

### 3.1.7 Command files

The control of IRIS can be carried out from within a command file set up by the user. This will enable complicated sequences of short runs which involve changing temperature, analyser configuration, chopper phase, etc. to be done automatically.

A command file can be created using one of the VMS editors and should ideally have the extension .COM to be consistent. An example command file is shown below (the comments would not be included in the real thing):

| | |
|---|---|
| $ CSET TEMP/VAL=10/LOLIMIT=8/HILIMIT=12/CONT | ! Set the temperature and define a range for data collection |

| | |
|---|---|
| $ PHASE6 8500 | ! Set the 6 m chopper phase to 8500 μs |
| $ PHASE10 12350 | ! Set the 10 m chopper phase to 12350 μs |
| $ LOAD [IRIS.CRPT]PG002.CRPT | ! Load the TCB information contained in file PG002.CRPT* |
| $ BEGIN | ! Begin the run |
| $ CHANGE TITLE """"Methyl pyridine at 10K PG002"""" | ! Change the title of the experiment |
| $ WAITFOR 200 uamps | ! Wait for 200 μamps of proton current |
| $ END | ! End the run |

* There are a number of standard .CRPT files for use in loading the appropriate TCB information for standard settings of the instrument.

### 3.2 Data visualisation and analysis

3.2.1 Interactive programs

GENIE - "A Language for Spectrum Manipulation and Display" [3] - is a software package common to all ISIS instrument and is used for displaying and manipulating spectra and data sets. Detailed information can be found in the GENIE manual available in the ICR and from the ISIS computer support group. A GENIE session can be started from the IRIS menu on the session manager window. The session consists of a graphics window and a command line window. The most commonly used commands are:

| | |
|---|---|
| >> **ASSign DAE** | all following operations will be carried out on the data currently being accumulated in the DAE i.e. you can look at the data in the DAE. |

| | |
|---|---|
| >> **ASSign 'NRUN'** | all following operations will be carried out on the data from run number 'NRUN' |
| >> **Display S1** | displays the data in spectrum number 1 (on IRIS this is the incident beam monitor) |
| >> **W1 = S3>S33** | adds together the data in spectra 3 to 33 and puts the result into workspace number 1 |
| >> **Display W1** | displays the data in workspace number 1 |

N.B. The commands are not case-sensitive

Typing PROGS inside GENIE will list the available programs for use within GENIE.

A new version of GENIE called OPENGENIE is being introduced. A copy of the manual for this software can be found on the WEB at:

"http://WWW.ISIS.RL.AC.UK/GenieUserManual".

ZEUS is an interactive data analysis and visualisation package available on the FEM only. It makes use of OPENGENIE and the PGPLOT graphical package but with a TK/TCL interface (buttons and slider-bars) which should make it more user-friendly. ZEUS is an item in the IRIS menu. It is still in development but should replace GENIE as the main way of inspecting data. Check with the local contact or instrument scientist on the current status.

IKON (a GENIE-lookalike) is used to convert the time-of-flight data into $S(Q,\omega)$. Detailed information is included in the IDA manual [3].

Most of this software apart from the ZEUS program can be accessed from an account on a VMS or OPENVMS machine by modifying the login.com to include the following lines:

```
$ IRIS:==@IRIS$DISK:[IRSMGR.PROGS]USER_LOGIN.COM
$ IF f$mode().nes."BATCH" then goto cont
$ IRIS
$ EXIT
$ CONT:
```

The necessary logical definitions will automatically be set up in batch mode and in interactive mode typing IRIS followed by carriage return will do the same.

### 3.2.2 Batch programs

IDA (IRIS Data Analysis) is a suite of programs for the analysis of IRIS data. Details of the programs can be found in the IDA manual. It can be run in two forms: a simple menu-driven system in a VMS/OPENVMS window; a Tk/TCL interface called IGIS (can be started from a VMS/OPENVMS window but on the FEM is an item in the IRIS menu).

## References


1. The design of the IRIS inelastic neutron spectrometer and improvements to its analysers. C J Carlile and M A Adams. Physica B 182 (1992) pp. 431-440.

2. PUNCH user guide. R G Parry et al. RAL Report, RAL 88109 (1988).

3. IDA - Iris Data Analysis. W S Howells. RAL Technical Report, RAL-TR-96-006. January 1996.

## Appendix I. Standard instrument settings

**Table 1** Inelastic settings

| Analyser reflection and relative intensity | Resolution (FWHM) at elastic line (μeV) | ΔE (meV) | Chopper operating frequency. | Time Channel Boundaries (μS) | Monitor boundaries (μS) | Computer command |
|---|---|---|---|---|---|---|
| PG002 (1.0) | 15.2 | -0.4 to 0.4 | 50 | 56000 - 76000 | 63000 - 65000 | PG002 |
| (1.0) | | -0.2 to 1.2 | 50 | 50000 - 70000 | 63000 - 65000 | PG002_OFFSET |
| (0.5) | | -0.8 to 0.8 | 25 | 50000 - 90000 | 63000 - 65000 | |
| (0.33) | | -1.0 to 10.0* | 16.7 | 22000 - 82000 | 63000 - 65000 | |
| PG004 (0.7) | 50.0 | -3.5 to 4.0 | 50 | 24000 - 44000 | 31000 - 33000 | PG004 |
| MICA002 (0.04) | 1.2 | -0.02 to 0.02 | 50 | 181000 - 201000 | 189000 - 191000 | MICA002 |
| MICA004 (0.15) | 4.5 | -0.15 to 0.15 | 50 | 86000 - 106000 | 94000 - 96000 | MICA004 |
| MICA006 (0.4) | 11.0 | -0.4 to 0.4 | 50 | 56000 - 76000 | 63000 - 65000 | MICA006 |

* Beryllium filter required - ask Instrument Scientist

If the computer commands are being used then it is necessary to first of all edit the appropriate .CRPT files in IRIS$DISK0:[IRIS.CRPT]. The names of the files are consistent with the commands e.g. PG002 and PG002.CRPT.

**Table 2** Diffraction Settings

| d-spacing range (Å) | Time-channel-boundaries (μS) | Monitor boundaries (μS) | D'n'.CRPT* | Computer command |
|---|---|---|---|---|
| 1.00 to 2.60 | 12500 - 52500 | 31000 - 33000 | n=1 | D1 |
| 2.20 to 3.80 | 38000 - 78000 | 51000 - 53000 | 2 | D2 |
| 3.40 to 5.10 | 60000 - 100000 | 71000 - 73000 | 3 | D3 |
| 4.60 to 6.40 | 83000 - 123000 | 101000 - 103000 | 4 | D4 |
| 5.90 to 7.40 | 105000 - 145000 | 121000 - 123000 | 5 | D5 |
| 7.00 to 8.70 | 128500 - 168500 | 151000 - 153000 | 6 | D6 |
| 8.30 to 9.90 | 151000 - 191000 | 171000 - 173000 | 7 | D7 |
| 9.60 to 11.00 | 173500 - 213500 | 191000 - 193000 | 8 | D8 |
| 10.75 to 12.50 | 195500 - 235500 | 221000 - 223000 | 9 | D9 |
| 11.80 to 13.40 | 216500 - 256500 | 231000 - 233000 | 10 | D10 |
| 12.80 to 14.44 | 235500 - 275500 | 251000 - 253000 | 11 | D11 |
| 14.07 to 15.70 | 260000 - 300000 | 275000 - 277000 | 12 | D12 |

* The files D'n'.CRPT (n=1,12) are located in the area IRIS$DISK0:[IRIS.CRPT] and contain the appropriate time channel boundary and monitor information for each of the d-spacing ranges specified in the table. They can be used to load this data automatically from within a command file (see the LOAD command in the PUNCH manual).

## Appendix II. Instrument parameters

Primary flight-path:

$L_1 = 36.40m$

Secondary flight-path:

$L_2 = 1.47m$ (Inelastic)

$L_2 = 0.825m$ (Elastic - nominal)

Angular coverage of ZnS detector banks:

$25° < 2\theta < 155°$

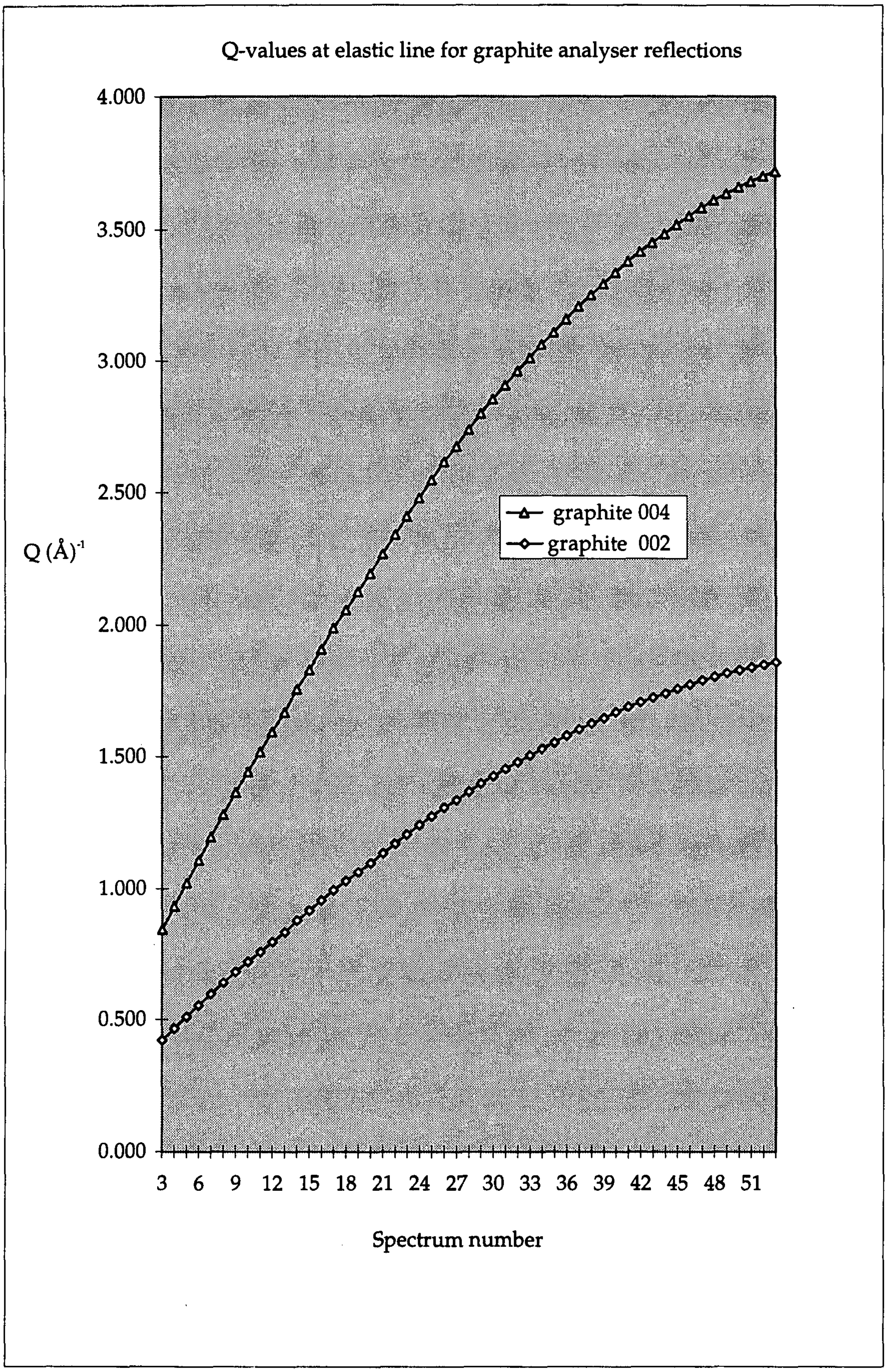
Angles of diffraction detectors:

$167.5° < 2\theta < 172.5°$

Operating vacuum:

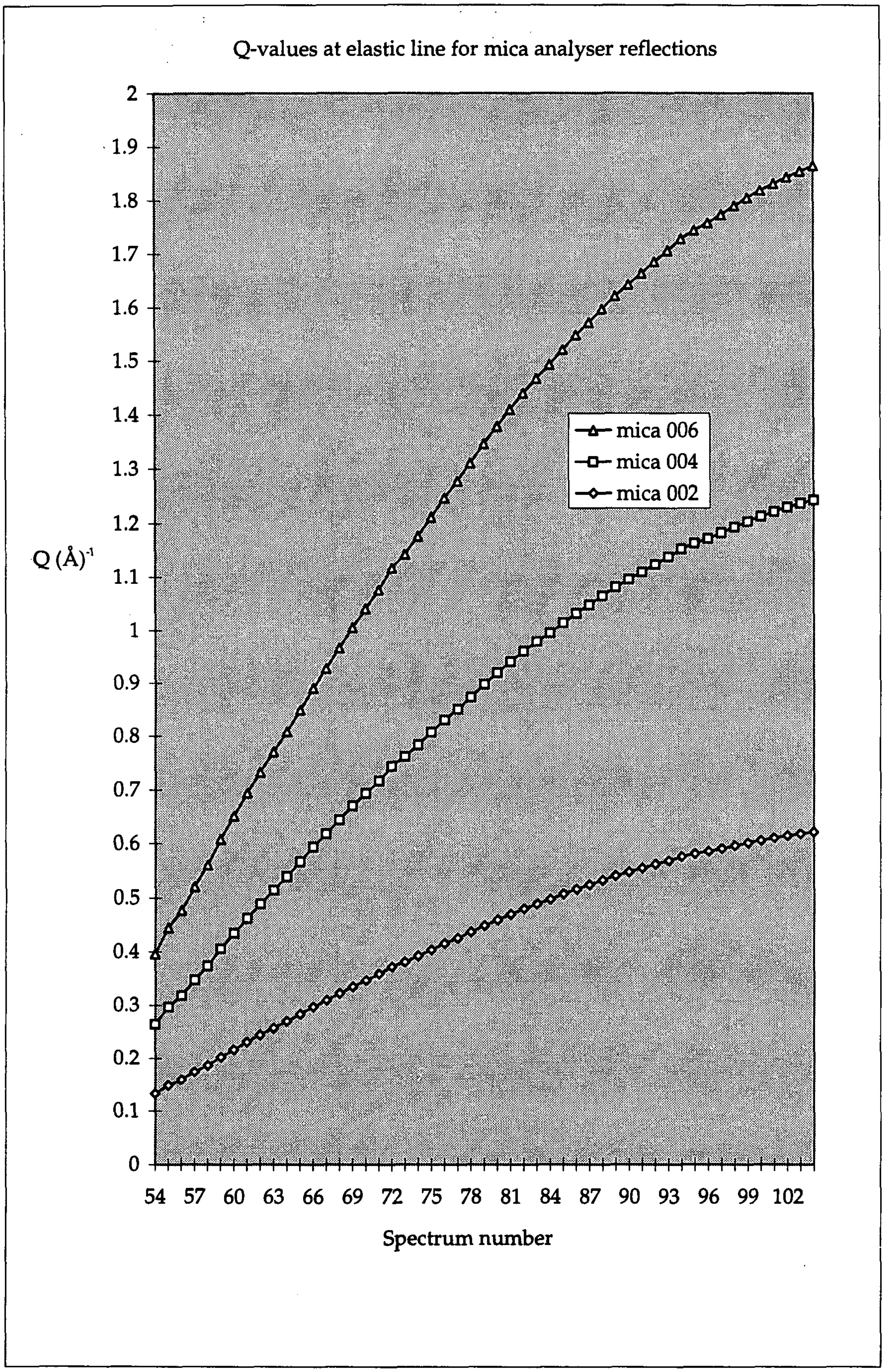
$5 \times 10^{-6}$ mbar in instrument tank

$1 \times 10^{-6}$ mbar in sample environment tank



Q-values at elastic line for graphite analyser reflections
4.000
3.500
3.000
2.500
2.000
1.500
1.000
0.500
0.000
Q (Å)-1
graphite 004
graphite 002
3 6 9 12 15 18 21 24 27 30 33 36 39 42 45 48 51
Spectrum number

| Spectrum Number | 2θ° | graphite 002 | graphite 004 |
|---|---|---|---|
| 3 | 25.75 | 0.422 | 0.844 |
| 4 | 28.50 | 0.466 | 0.933 |
| 5 | 31.25 | 0.510 | 1.020 |
| 6 | 34.00 | 0.554 | 1.108 |
| 7 | 36.75 | 0.597 | 1.194 |
| 8 | 39.50 | 0.640 | 1.280 |
| 9 | 42.25 | 0.683 | 1.365 |
| 10 | 44.75 | 0.721 | 1.442 |
| 11 | 47.25 | 0.759 | 1.518 |
| 12 | 49.75 | 0.797 | 1.594 |
| 13 | 52.25 | 0.834 | 1.668 |
| 14 | 55.25 | 0.878 | 1.757 |
| 15 | 57.75 | 0.915 | 1.829 |
| 16 | 60.50 | 0.954 | 1.909 |
| 17 | 63.25 | 0.993 | 1.987 |
| 18 | 65.75 | 1.028 | 2.056 |
| 19 | 68.25 | 1.062 | 2.125 |
| 20 | 70.75 | 1.096 | 2.193 |
| 21 | 73.50 | 1.133 | 2.267 |
| 22 | 76.25 | 1.169 | 2.339 |
| 23 | 79.00 | 1.205 | 2.410 |
| 24 | 81.75 | 1.239 | 2.479 |
| 25 | 84.50 | 1.273 | 2.547 |
| 26 | 87.25 | 1.307 | 2.614 |
| 27 | 89.75 | 1.336 | 2.673 |
| 28 | 92.50 | 1.368 | 2.737 |
| 29 | 95.25 | 1.399 | 2.799 |
| 30 | 97.75 | 1.427 | 2.854 |
| 31 | 100.25 | 1.453 | 2.907 |
| 32 | 102.75 | 1.480 | 2.960 |
| 33 | 105.25 | 1.505 | 3.011 |
| 34 | 107.75 | 1.530 | 3.060 |
| 35 | 110.25 | 1.554 | 3.108 |
| 36 | 113.00 | 1.579 | 3.159 |
| 37 | 115.75 | 1.604 | 3.208 |
| 38 | 118.25 | 1.625 | 3.252 |
| 39 | 120.75 | 1.646 | 3.293 |
| 40 | 123.50 | 1.668 | 3.337 |
| 41 | 126.25 | 1.689 | 3.379 |
| 42 | 128.75 | 1.708 | 3.416 |
| 43 | 131.25 | 1.725 | 3.451 |
| 44 | 133.75 | 1.742 | 3.484 |
| 45 | 136.50 | 1.759 | 3.519 |
| 46 | 139.25 | 1.775 | 3.551 |
| 47 | 142.00 | 1.791 | 3.582 |
| 48 | 144.75 | 1.805 | 3.611 |
| 49 | 147.25 | 1.817 | 3.635 |
| 50 | 150.00 | 1.829 | 3.659 |
| 51 | 152.75 | 1.841 | 3.682 |
| 52 | 155.25 | 1.850 | 3.700 |
| 53 | 158.00 | 1.859 | 3.719 |


Q-values at elastic line for mica analyser reflections
Q (Å)-1
Spectrum number
mica 006
mica 004
mica 002
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2
54 57 60 63 66 69 72 75 78 81 84 87 90 93 96 99 102

| Spectrum Number | 2θ° | mica 002 | mica 004 | mica 006 |
|---|---|---|---|---|
| 54 | -24.00 | 0.132 | 0.264 | 0.396 |
| 55 | -27.00 | 0.148 | 0.296 | 0.444 |
| 56 | -29.00 | 0.159 | 0.318 | 0.477 |
| 57 | -31.75 | 0.174 | 0.347 | 0.521 |
| 58 | -34.25 | 0.187 | 0.374 | 0.561 |
| 59 | -37.25 | 0.203 | 0.405 | 0.608 |
| 60 | -40.00 | 0.217 | 0.434 | 0.651 |
| 61 | -42.75 | 0.231 | 0.463 | 0.694 |
| 62 | -45.25 | 0.244 | 0.488 | 0.732 |
| 63 | -47.75 | 0.257 | 0.514 | 0.771 |
| 64 | -50.25 | 0.269 | 0.539 | 0.808 |
| 65 | -53.00 | 0.283 | 0.566 | 0.850 |
| 66 | -55.75 | 0.297 | 0.593 | 0.890 |
| 67 | -58.25 | 0.309 | 0.618 | 0.927 |
| 68 | -61.00 | 0.322 | 0.644 | 0.966 |
| 69 | -63.75 | 0.335 | 0.670 | 1.005 |
| 70 | -66.25 | 0.347 | 0.694 | 1.040 |
| 71 | -68.75 | 0.358 | 0.717 | 1.075 |
| 72 | -71.75 | 0.372 | 0.744 | 1.116 |
| 73 | -73.75 | 0.381 | 0.762 | 1.143 |
| 74 | -76.25 | 0.392 | 0.784 | 1.175 |
| 75 | -79.00 | 0.404 | 0.807 | 1.211 |
| 76 | -81.75 | 0.415 | 0.831 | 1.246 |
| 77 | -84.25 | 0.426 | 0.851 | 1.277 |
| 78 | -87.00 | 0.437 | 0.874 | 1.311 |
| 79 | -90.00 | 0.449 | 0.898 | 1.346 |
| 80 | -92.75 | 0.459 | 0.919 | 1.378 |
| 81 | -95.50 | 0.470 | 0.940 | 1.409 |
| 82 | -98.25 | 0.480 | 0.960 | 1.440 |
| 83 | -100.75 | 0.489 | 0.978 | 1.467 |
| 84 | -103.25 | 0.498 | 0.995 | 1.493 |
| 85 | -106.00 | 0.507 | 1.014 | 1.521 |
| 86 | -108.75 | 0.516 | 1.032 | 1.548 |
| 87 | -111.25 | 0.524 | 1.048 | 1.571 |
| 88 | -114.00 | 0.532 | 1.065 | 1.597 |
| 89 | -116.75 | 0.540 | 1.081 | 1.621 |
| 90 | -119.25 | 0.548 | 1.095 | 1.643 |
| 91 | -121.75 | 0.554 | 1.109 | 1.663 |
| 92 | -124.50 | 0.562 | 1.123 | 1.685 |
| 93 | -127.25 | 0.569 | 1.137 | 1.706 |
| 94 | -130.25 | 0.576 | 1.152 | 1.727 |
| 95 | -132.75 | 0.581 | 1.163 | 1.744 |
| 96 | -134.75 | 0.586 | 1.172 | 1.757 |
| 97 | -137.25 | 0.591 | 1.182 | 1.773 |
| 98 | -140.00 | 0.596 | 1.193 | 1.789 |
| 99 | -142.75 | 0.601 | 1.203 | 1.804 |
| 100 | -145.50 | 0.606 | 1.212 | 1.818 |
| 101 | -148.25 | 0.610 | 1.221 | 1.831 |
| 102 | -151.00 | 0.614 | 1.229 | 1.843 |
| 103 | -153.75 | 0.618 | 1.236 | 1.854 |
| 104 | -156.50 | 0.621 | 1.243 | 1.864 |

## APPENDIX III. Out of hours support

Normal working hours for most staff (apart from the ISIS crew who are on shift duty) are from 08:30 until approximately 17:00, Monday to Friday. Outside these hours most local contacts at ISIS, which includes those on IRIS, and most members of the technical support groups voluntarily agree to provide some form of assistance to users. Usually this is, in the first instance, a telephone number where they may be contacted if problems occur. A list of the relevant telephone numbers is available in the ICR. The first point of call (after this manual) should be the local contact for the experiment.

This assistance is available during "reasonable times". The definition of what is reasonable depends upon the individual concerned and should be determined before calling if at all possible. As a general rule, for local contacts on IRIS and members of the technical support groups, the hours between 08:00 and 23:00 would probably be considered reasonable. Unless it has been previously agreed that a person may be contacted outside of these hours then in normal circumstances outside of these hours the following procedure should be adopted:

1) Check the manual for possible solutions and explanations.

2) Investigate whether the problem can be put off until a more reasonable time - for example, whether the experimental timetable can be adjusted by, perhaps, performing a background or a resolution run.

3) Check whether a member of the ISIS crew is able to assist with the problem.

4) If none of the above applies then ensure that the experimental set-up is safe (the ISIS duty officer will be able to advise if necessary) then leave it and wait until a more reasonable time. Loss of beamtime due to ISIS/IRIS/Sample Environment problems is **always** dealt with sympathetically and if appropriate the beamtime is recouped at a later date, if this is possible.

## APPENDIX IV. Useful telephone numbers

General:

| | |
|---|---|
| Accident/Emergency/Fire | 2222 |
| Health Physics (Radiation) | 6696 |
| ISIS Main Control Room (MCR) | 6789 |
| IRIS Control Room (ICR) | 6836 |
| Main gate (Security) | 5545 |
| Computer support | 3029/5414 |

Office numbers :

| | |
|---|---|
| Instrument Scientist - | |
| Mark Adams | 6157 |
| Local contacts - | |
| Spencer Howells | 5680 |
| David Martin | 6157 |
| Winnie Kagunya | 5797 |
| Richard Ibberson | 5871 |
| Toby Perring | 5428 |
| Roger Eccleston | 5409 |