Proc. Int. Symposium on Neutron Optics and Related Research Facilities, Kumatori, 1996
J. Phys. Soc. Jpn. **65** (1996) Suppl. A pp. 245-248

The Osiris Polarisation Analysis Spectrometer and Diffractometer

D. Martín, *S. Campbell and C. J. Carlile

ISIS Pulsed Source, Rutherford Appleton Laboratory, Chilton, Didcot, UK
**Department of Pure and Applied Physics, University of Salford, Salford, UK*

(Received 6 March 1996; accepted 21 March 1996)

The Osiris Project will explore the possibilities for cold neutrons on pulsed sources using a versatile approach that will allow structural and dynamical studies of condensed matter by several methods ranging from unpolarised neutron scattering to full polarisation analysis. The instrument is situated at the end of a supermirror guide with a final converging section. The first options to be implemented are a large powder diffraction detector in near backscattering geometry and a multiple crystal analyser with its corresponding detectors in inverted geometry. Monte Carlo simulations of the neutron guide will be presented.

KEYWORDS: Neutron Instrumentation, Computer Simulations, Polarised Neutrons.

§.1. Introduction

The Osiris Project will explore the instrumental horizons available with the cold neutrons from a pulsed source and especially the totally new avenues available to polarised neutrons on these sources. Pulsed neutron sources offer opportunities which reactor facilities cannot. Some instruments with partially polarised incident-beams and full polarisation analysis exist on reactor sources but with modest resolution. However on pulsed sources, polarisation techniques offer great potential for high resolution studies and only lack of opportunity has left the field unexploited. The fundamentally novel methods developed on IRIS[1] will be combined with proven and extended neutron polarising techniques. The pioneering work of Endoh and collaborators[2] has demonstrated the feasibility of optical polarization for cold neutrons on pulsed sources, and the high flux available at ISIS, coupled to the advanced design of the Osiris guide will provide the means to take this field to its next evolutionary stage. By exploiting the combination of sharp pulses, white beams and cold neutrons from ISIS, high resolution measurements, both dynamic and structural, can be carried out using both unpolarised and polarised neutrons.

The Osiris Project is an international collaboration with the participation of India, Spain, Sweden, Switzerland and the United Kingdom. Due to its open character more countries have already expressed their interest, such as Italy for example, who are expected to join the project in the near future.

The project has three well-defined phases:

- *Phase I*
  --Extraction of a second cold beam guide from the IRIS beam line
- *Phase II*
  --Large d-spacing powder diffraction
  --Incident beam polarised powder diffraction
- *Phase III*
  --High resolution spectroscopy
  --Spectroscopy polarisation analysis
  --Diffraction polarisation analysis

Correspondence to: D. Martín, ISIS Pulsed Source, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK.

The first two phases are already at an advanced stage, with *Phase I* reaching completion by the end of April 1996 and *Phase II* during the last cycle of 1996, with the first neutron diffraction patterns being recorded. The first stages of *Phase III* are at an advanced design stage.

This paper will give a brief description of *Phases II* and *III* and then concentrate in the design of the neutron guide.

§.2. Design

Viewing a 25K liquid hydrogen moderator, the Osiris primary flight path starts from the same beam hole as IRIS, N6, in such a geometry that no reduction in intensity at the IRIS sample position is caused. This is the first time such an approach has been used at ISIS and will eventually play an important role in the design of future pulsed sources such as the European Spallation Source. The neutrons spectrum has an appreciable intensity in the range [$1\text{Å} \le \lambda \le 30$ Å] and it is intended to transmit as much as possible of this intensity to the sample position by means of a supermirror guide with m=2 and a converging section with m=4, where m=1 is the critical angle of nickel per unit wavelength. Two disk choppers at 6.3 and 10 metres from the moderator, eliminate frame overlap of succeeding pulses and allow a wavelength band of 2Å, to be delivered to the sample when the choppers are run at the ISIS frequency of 50Hz.

2.1. The Diffractometer

The exploratory measurements carried out on IRIS with long wavelength diffraction in backscattering geometry demonstrates that the 25 K hydrogen moderator provides an enhanced flux with useful intensity up to 30Å. This incident flux will even be larger on Osiris as is shown in Fig.1.

The resolution will be excellent and almost constant in the important range above 2.35Å, where the aluminium windows become transparent. This excellence is due to the fact that at long wavelengths the dominant contributions to the resolution are two: the moderator pulse width and the cot $\theta \cdot \Delta\theta$ term of the angular resolution. The moderator pulse width remains unchanged at 120μsec after the peak of the maxwellian, matching the angular contribution around 10 Å. This powder diffraction detector consists of a one meter diameter circular bank of scintillators centred at

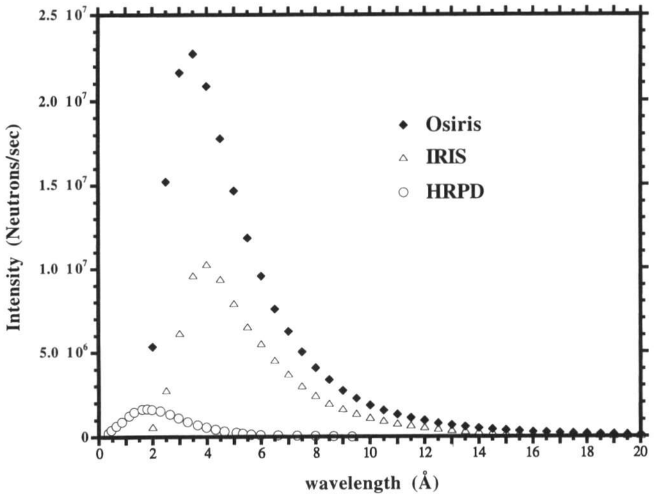

Fig. 1. Neutron intensity at the exit of HRPD, IRIS and Osiris as a function of wavelength. HRPD and IRIS results are measured intensities. Osiris results are Monte Carlo simulations.

Table I. Diffractometer Specifications

Solid angle	0.67 ster
Scattering angle range	$[150° \leq 2\Theta \leq 175°]$
Resolution($\Delta d/d$)	2.5×10^{-3}
d-spacing range	$[1 \leq d \leq 15]$Å

Table II. Spectrometer Specifications

Analysing energy PG(002)	1.82 meV
Energy transfer range	$[0.8 \leq \Delta E \leq 5]$meV
Scattering angle range	$[5° \leq 2\Theta \leq 160°]$
Momentum Transfer	$[0.1 \leq \Delta Q \leq 1.8]$Å^{-1}
Resolution	25 μeV

the sample position. Its specifications are given in Table I.

The solid angle of the detector is 50 times larger than the present IRIS detector, promising a count rate increase of two orders of magnitude.

2.2. The Spectrometer

White beam crystal analyser spectroscopy inverts the (Q, ω) space available within which to observe dynamical processes, compared with direct geometry instruments. This has the consequence that high resolution spectra can still be recorded at high energy transfers with the sample cold and in its ground state without contamination from higher excited states. This has been fully exploited on IRIS and the extremely good results, especially in the interpretation of complex spectra, have been a paramount criterion in the selection of Osiris spectrometer geometry.

The Osiris Project spectrometer will consists of a pyrolytic graphite multiple crystal analyser cooled to 4K. It comprises a mosaic of approximately 5000 individual crystals and has an approximate height of 20cms, a length of 250cms and is situated on the arc of a circle approximately 80cms from the sample. The detectors are 5cm long helium tubes situated in near backscattering position with respect to the crystals: 170 degrees. The calculated characteristics of the spectrometer are given in Table II.

2.3. Polarised Neutrons

Before the converging final section of the neutron guide, a set of three polarisers, a bender collimator (mirroring one of the collimators) and a supermirror guide section can be positioned. This approach ensures a great degree of versatility, since the most appropriate polariser can be chosen for the required wavelength range. The collimator ensures the possibility of checking the effect of the polariser used in the spectrometer, and the removable guide section permits non-polarised neutrons to reach the sample. The polarising neutron benders, multilayers of cobalt and titanium, are initially magnetized longitudinally and the remanence is kept at a high level by means of individual solenoids.

In both cases, diffraction and spectroscopy, full polarization analysis is possible by positioning another set of Soller polarising benders in the scattering path after the sample. For diffraction this is straightforward by simply using polarisation analysers in front of the detector, but for spectroscopy the neutrons will go through the polarisation analyser twice, before and after reflection by the graphite crystal analyser. This solution is necessary to ensure a high degree of polarisation and to preserve the backscattering high resolution geometry but at the expense of a significant reduction in intensity. Both paths, primary and secondary, are provided with their corresponding spin flippers.

Vectorial polarisation analysis will be achieved by the spin rotator method.[3] Adiabatic rotation of the polarisation direction in the three orthogonal directions is conducted in the space volume around the sample by means of magnetic fields provided by removable Helmholtz coils. Their field strength can be adjusted as a function of the neutron wavelength to ensure the adiabaticity of the process without changing the sample magnetization.

§.3. The Neutron Guide

At the core of the Osiris project lies its neutron guide. The high resolution expected from the instrument, coupled with the use of polarized neutrons, either with polarized incident beam or full polarisation analysis, can only be achieved if the neutron flux at the sample position is enhanced to a level never before achieved with cold neutrons on a pulsed source. Three steps are necessary to reach this goal:

- Increasing the critical angle of the guide.
- Reducing the losses.
- Increasing the flux.

All of the above steps were optimized by means of Monte Carlo simulations of the guide.

3.1. Increasing the critical angle

A neutron impinging on a surface experiences the total reflection phenomenon equivalent to the effect experienced by light. Analogous definitions are used and the critical angle γ_c is defined as the largest angle below which total reflection takes place. Above this angle neutrons are not reflected, but are transmitted or absorbed through the surface. Theoretically, below γ_c the reflectivity is 100% and above it 0%. γ_c is a function of the neutron wavelength λ and the coherent scattering density $\overline{N}\,\overline{b}$ of the coating of the surface:

$$\frac{\gamma_c}{\lambda} = \sqrt{\frac{\overline{N}\,\overline{b}}{\pi}} \qquad (3.1)$$

The highest critical angle per unit wavelength at a reasonable price is achieved with nickel with γ_c / λ = 0.00173, rad/Å. In the literature this value is known as m = 1 and as an example, the IRIS guide is made with such a coating, except for the last converging section.

The Osiris guide has a supermirror coating with m = 2. Supermirror coatings are made of a sequence of multilayers of two different materials inducing a Bragg reflection effect[4] that increases the available critical angle, although with a reduction in reflectivity after m = 1. Depending on the wavelength the increase of intensity can be dramatic, reaching up to three fold the value obtainable with a normal nickel coating.

This increase in γ_c was also achieved in the crucial section closest to the tantalum target: the shutter. But the high radiation levels in this section preclude the use of normal glass guides. Instead stainless steel is used (as in IRIS) which is inadequate for a supermirror coating as will be explained below. Consequently the increase in γ_c for this section was possible only by the use of supermirror coated glass panels attached to the steel cavities. If this novel solution is succesful in the medium and long term, it will be the model to follow by the future European Spallation Source.

3.2. Reducing the losses

The reflectivity of a supermirror coating is highly dependent on the morphology of the underlaying surface.[5] This morphology changes with the nature of the glass used as substrate (float, borated, polished, etc.) and, for each type of glass, with the manufacture batch and company. When a high intensity of neutrons is necessary as in the Osiris case, just choosing a provider of supermirror guides is not a reliable method. Instead the batch of coated glass is chosen *after* its reflectivity has been measured using the microguide technique, originally developed at the Bhabha Atomic Research Centre in Bombay, India. A very precise device was built for this purpose and it can be run concurrently with the IRIS spectrometer as a parasitic instrument extracting 6.27Å, neutrons by means of a pyrolytic graphite crystal placed in the neutron guide. The multi-reflectivity is then measured and the reflectivity extracted from it. Only those batches with a reflectivity above 86% at the m = 2 edge are allowed in the construction of the guide.

3.3. Increasing the flux

The 4.3×6.5 cms cross section of Osiris supermirror guide will provide a high intensity at the sample provided the sample is large enough! The question that has to be tackled therefore, is an increase of the *flux* in order to be able to use a realistic sample size. More important, for diffraction experiments a small and narrow sample is desirable if the expected resolution is to be obtained. Using a supermirror converging guide is the straightforward solution for a nickel coated guide as is done on IRIS. The situation is different if the main body of the guide has m = 2 already. As a consequence the converging guide needs a coating with

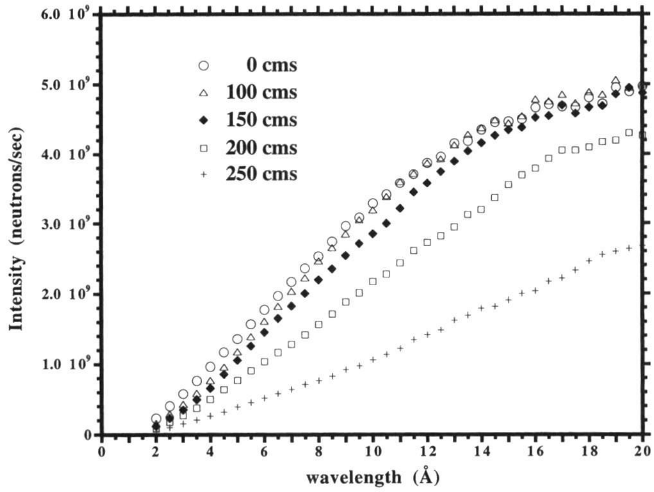

Fig. 2. Neutron intensity at sample position as a function of wavelength and length of converging guide. Constant sample size: 6.5×4.3 cms.

m = 4 to be fully effective, which has not been achieved at the time of the guide design! The modular approach of Osiris design allows to experiment with new developments. The converging guide is susceptible of being removed easily as advances in supermirror techniques appears. In fact at the time of writing, a team lead by P. Böni from the PSI has already achieved such a supermirror.[6] The walls of the converging guide are inclined by an angle of 0.00692 rad to the central axis of the beam, i.e. it is seen as straight for 2Å neutrons.

After the angle of inclination for the converging guide has been decided, its length has to be optimised to maximize the flux at the sample position without a significant reduction in total intensity over the sample. The process was done using a modified version of the program MCGUIDE.[7] Results of these simulations are shown in Fig.2.

Two important points to highlight resulting from the simulations:

- The main cause of neutron loss is due to the low reflectivity of the converging guide beyond m = 2. The approach normally used for a nickel guide with a converging guide of m = 2 includes the use of a long converging guide to reduce the steepness of the tapering angle, which in turn reduces the amount of neutrons with a take-off angle larger than the critical. This approach should be abandoned when the converging guide has a high value of m since the losses due to low reflectivity are higher than those caused by higher than critical angle reflections.
- At the end of the curved section of a nickel guide, a straight section is normally added to reduce the asymmetry of the beam at the guide exit. This asymmetry caused by the accumulation of neutrons on the outer side of the guide is reduced to an insignificant value in a supermirror guide eliminating the need of the straight section and therefore relaxing the curvature of the guide with the associated increase of neutrons at guide exit.

After a lengthy iterative process, the guide design optimised to the needs of Osiris was determined. Its characteristics are described in Table III.

§.4. Conclusions

The modular approach of the Osiris project will allow a wide range of scientific applications to be explored, establishing the foundations for the European Spallation Source new instrumentation. The foreseeable scientific areas in the near future may be distributed amongst two operational modes: spectrometer and diffractometer.

Spectrometer

Non-polarised mode: molecular dynamics and diffusional processes in solids and liquids, low energy inelastic scattering from magnetic excitations and quantum tunnelling phenomena. Separation of magnetic excitations and nuclear excitations of ferromagnets when the incident beam is polarised and in antiferromagnetic and paramagnetic samples in full polarisation mode. Distinction of quasielastic and low energy inelastic coherent contribution from incoherent contribution in pure isotopes.

Diffractometer

In the non-polarised mode of operation the diffraction detector allows for long d-spacing diffraction and the study of very large unit cells structures up to 100,000Å^3 as well as kinetic studies of phase transitions and chemical reactions. Magnetic superstructures and small biomolecular and pharmaceuticals will benefit. With the incident beam polarised it is possible to identify magnetic scattering by the sample, enabling the study of magnetic multilayers and ferromagnetic samples. In full polarisation mode the separation of magnetic scattering from nuclear scattering can be achieved in antiferromagnetic and paramagnetic samples. Determination of coherent and incoherent contributions to the structure factor in the absence of isotopic incoherent contribution, will also be possible.

Acknowledgments

The authors kindly acknowledge extremely useful discussions with Dr. O. Schärpf (ILL) and Dr. P. Böni (PSI) who provided their expertise in the fields of polarised neutrons and supermirror coatings respectively. Thanks are given to Dr. J. Penfold and Mr. M. Adams (both from ISIS) for their kind provision of measuring time on CRISP and SURF, and IRIS. Work done by D. Martín was supported during 1993 and 1994 by a grant from the European Union under the Human Capital and Mobility Program with contract: ERB-CHBGCT920194 and during 1995 and 1996 by spanish grant from C.S.I.C. Convocatoria BOE 30-05-94. S. Campbell work was supported by awarded Ph.D. grant number 94302560 from EPSRC (UK).

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Table III. Osiris guide details

Length (cm)	Width (cm)	Height (cm)	R. of C. (km)	γ_c/λ rad/Å
150.0	4.5	6.7	∞	0.00346
46.8	4.5	6.7	∞	0.00346
7.85	4.5	6.7	∞	Gap
200.0	4.3	6.5	∞	0.00346
43.0	4.3	6.5	∞	0.00346
11.75	4.3	6.5	∞	Chopper
300.0	4.3	6.5	2.05	0.00346
68.2	4.3	6.5	2.05	0.00346
7.56	4.3	6.5	2.05	Chopper
2100.0	4.3	6.5	2.05	0.00346
64.39	4.3	6.5	2.05	0.00346
1.15	4.3	6.5	∞	Gap
50.0	4.3	6.5	∞	0.00346
3.0	4.3	6.5	∞	Monitor
150.0	4.3 → 2.2	6.5 → 4.4	∞	0.00692