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Optimisation of PRISMA at ISIS for cold neutron single crystal spectroscopy

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ABSTRACT

The PRISMA spectrometer at ISIS is being developed into an instrument optimised for cold neutron single crystal spectroscopy. The conversion of the beamline to accept interchangeable detector modules is complete and the current layout of the instrument and detector systems is described. The second phase of the development will be the installation of a supermirror neutron guide that will increase the cold neutron flux by factors of up to 20, with a corresponding impact on the scope of the scientific programme. The implications for the final guide design of several example beamline configurations evaluated by Monte Carlo calculations are discussed.

1. Introduction

The PRISMA indirect geometry crystal analyser spectrometer at ISIS has been operational for 10 years, and has proved to be particularly successful for overview experiments in single crystals in the thermal neutron energy range 20 - 80 meV and also for diffuse and critical scattering studies. Over the past 4 years, PRISMA has been converted into a modular instrument with a suite of three interchangeable detector modules allowing significantly greater experimental flexibility: (i) the original single-analyser system, (ii) a new high resolution double-analyser system, and (iii) a high resolution diffraction detector. The double-analyser system has been highly successful at obtaining high energy and wavevector resolution for analysing energies between 2 meV and 14 meV and is the first stage in the optimisation of PRISMA for cold neutron experiments. The beamline is to be further developed through the installation of a supermirror neutron guide leading to incident flux increases of factors between 10 and 15 for neutrons between 1 meV and 10 meV that will consequently allow new scientific areas to be opened up and will make PRISMA competitive with the best cold source triple axis spectrometers at reactor sources (which are already heavily oversubscribed). This work is being carried out within an R&D network for Cold Neutron Optimisation supported by the EU TMR-RTD programme. The development ties in strongly with the recommendations for R&D projects identified by the ESS technical feasibility study, particularly in the improvement of neutron optics and focussing devices, and the exploitation of cold neutrons at spallation sources for single crystal spectroscopy [1].

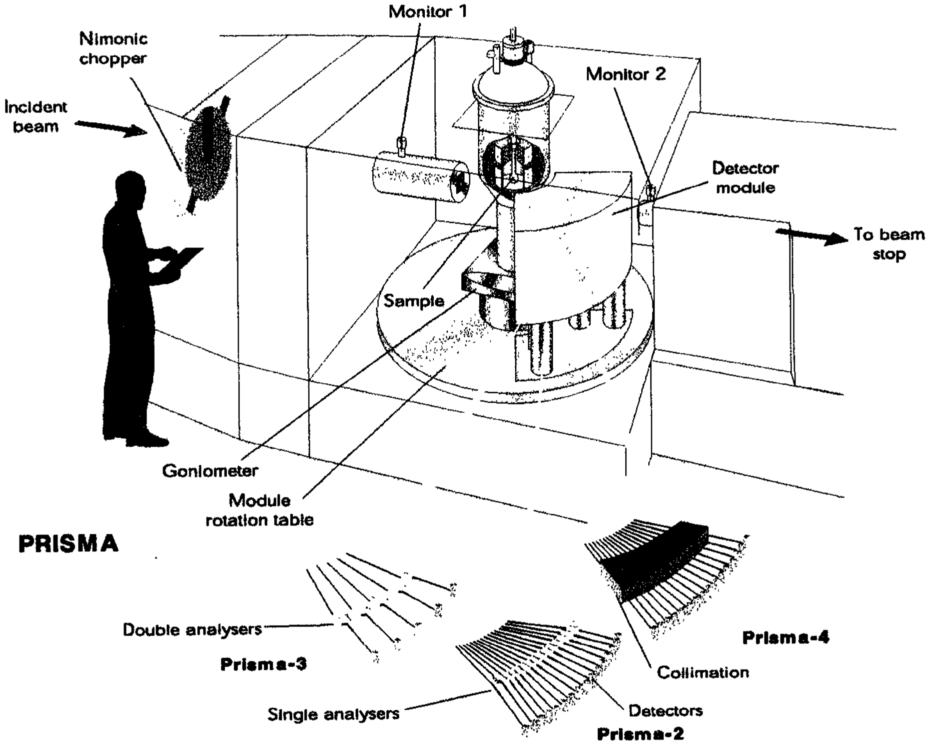

Figure 1 Schematic drawing of the PRISMA sample area

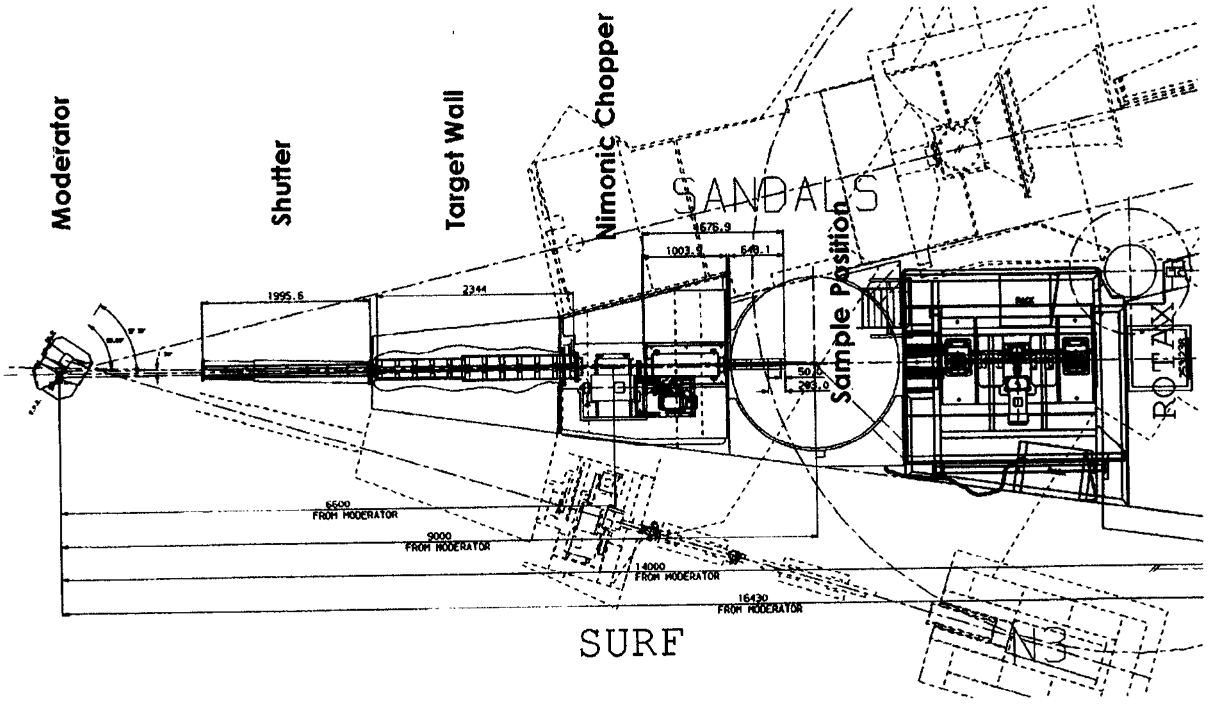

Figure 2 Engineering layout of the PRISMA beamline

2. Conversion to a modular instrument

PRISMA was originally designed to operate with final energies in the thermal energy range 20-50 meV [2] with an array of 16 analyser-detector arms separated by 2° in ϕ providing a close spacing of the TOF detector trajectories in reciprocal space. Whilst many successful experiments were performed with this arrangement, the continued and increasing interest in low energy excitations required considerably lower final energies in the cold neutron range 1-12 meV to obtain good resolution. However, to obtain $E_f < 12$ meV with the (002) reflections of a pyrolytic graphite (PG) analyser, the detector must be positioned at a scattering angle $2\theta_A > 50°$, an unattainable situation with the single-analyser detector system since adjacent detector arms collide. To overcome this mechanical constraint, a new high resolution low-E_f detector system has been constructed, requiring the parallel conversion of the original spectrometer into a modular instrument by rebuilding the beamline shielding around the sample area.

A schematic drawing of the PRISMA sample area is shown in Figure 1. A goniometer allows sample environment equipment to be oriented in the beam, and detector systems enclosed in individual shielding modules are mounted on a rotating table centred on the sample position. Removable roof shielding allows detector modules to be interchanged on a time scale of around 8 hours. The arrangement of the remaining beamline components are shown in the engineering layout of Figure 2. PRISMA views a 100 K methane moderator at 90° with the sample position located at a distance of 9.035 m. A 2 m thick steel shutter is located immediately outside the ISIS target vessel (1.714 m from the moderator) followed by 2 m of target wall shielding and a 50 Hz nimonic background chopper to block the epithermal flux from the moderator with a cadmium tail cutter to reduce the background from neutrons arriving after 12 ms in each 20 ms ISIS frame. The incident beam collimation is castellated with sintered B_4C edges surrounded by iron shot, B_4C and resin giving a horizontal divergence of 30' and a vertical divergence of 60' with a beam exit cross-section of 3 x 5 cm (width x height) at the sample position. Note that immediately behind PRISMA is the shutter of the ROTAX powder diffractometer and that the SURF reflectometer and SANDALS diffractometer are located on either side.

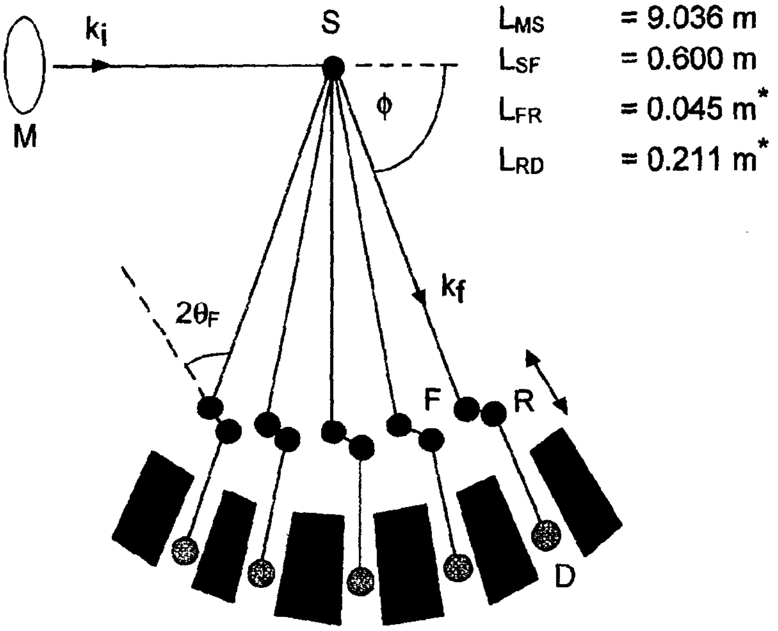

Figure 3 Schematic view of the double-analyser detector system. Starred lengths are defined when L_{FR} is at 90° to L_{SF}.

The high resolution, low-E_f detector module, Figure 3, contains five double-analyser detector arms each consisting of Soller collimation, two PG analyser crystals and a Reuter-Stokes 10 atm 1/2" ^{3}He gas detector [3,4]. The analyser arms are separated by 10° in ϕ, but a sequence of interleaving data sets can be collected for finer reciprocal space coverage. E_f is set by aligning both analysers to the appropriate Bragg angle with respect to the scattered beam direction, whilst the rear analyser is additionally mounted on a translation unit permitting movement towards or away from the fixed detector to maximise the signal. This arrangement gives an energy resolution $\Delta E_f / E_f \approx 4\%$ with final collimation 60'-open for $E_f < 12$ meV. With such low final energies, the overlap of the signal from λ and $\lambda/2$ reflections becomes significant and sets of PG or beryllium filters are available if required. Since there is no direct path from the sample to the detectors, an additional alignment detector consisting of five squashed ^{3}He tubes has also been constructed in a fixed 90° position. This reduces the time required for sample alignment and allows measurements of lattice parameters and d-spacings to be easily made during experiments.

In addition to the two inelastic detector modules, a third high resolution diffraction module is also available, optimised for diffuse scattering and critical scattering studies with 10' collimation [5]. Because of the small size of this module, it can be installed simultaneously with the double-analyser system, allowing inelastic and elastic data to be collected in the same experiment.

3. Improving the flux

The second stage in the optimisation of PRISMA will be the installation of a supermirror neutron guide between the target void vessel and the sample area. The close proximity of the instruments surrounding PRISMA imposes tight constraints upon the design options, the most significant being that the guide must be straight or tapered since there is insufficient space to install a curved guide.

```
1000000 1 0 8.0
[moderator]                   % 100 K methane moderator
9.035 0.0 0.0 0.1 0.1 0.0
95. 37.15 9.0 39.1
[guide]                       % shutter section
300 1
7.320 0.0 0.0 0.062 0.086
5.321 0.0 0.0 0.050 0.070
[guide]                       % target wall section
300 1
5.320 0.0 0.0 0.050 0.070
2.821 0.0 0.0 0.036 0.051
[chopper]                     % nimonic chopper
2.421 0.0 0.0 0.040 0.060
300.0 10300.0 20000.0
[soller]                      % chopper to sample pit
1 1
2.820 0.0 0.0 0.036 0.051
0.421 0.0 0.0 0.036 0.051
[area]                        % PRISMA sample position
50 50
0.000 0.0 0.0 0.125 0.125
[monitor]
[stop]
```

Figure 4 A typical PRMON input file. The first line specifies the number of neutrons and whether the neutron will be emitted towards the first element with a fixed or random energy defined by the flux shape in the moderator component. Each component is defined by its distance from the sample position, displacement from the central axis of the beam, and its width and height, with other parameters as required. Area detector components allow the flux distribution to be viewed, and monitor components record the time of flight profile of transmitted neutrons.

One advantage of this design is that experience will be gained with a considerably different guide system to those already existing at ISIS on the IRIS, OSIRIS and HRPD instruments.

To assess the parameters for the guide design, we are using a generalised Fortran Monte Carlo code PRMON developed by Mark Hagen. Components such as neutron guides, Soller collimation, nimonic choppers, area detectors or monitors can be assembled in any order to model a particular beamline configuration. A typical input file is shown in Figure 4. Simulation of the secondary part of the spectrometer including scattering from a sample is under development. Extensive testing of the code comparing simple beamline arrangements with analytical calculations has been carried out with excellent agreement found between the two methods. Here, six examples that illustrate the influence of various parameters upon the neutron intensity at the sample position are considered. The results of the calculations are summarised in Table 1 with the intensity at the ROTAX sample position also listed (ROTAX has 3 cm x 5 cm straight collimation through its shutter). Fixed beamline parameters included in the calculations are the 9.035 m moderator to sample distance, the 10 x 10 cm^2 moderator size and orientation of the beamline with respect to this, and the inclusion of a 0.75 m gap to accommodate the nimonic chopper. For these calculations, guide sections all have m = 3 supermirrors and intensities have been normalised to the exit beam area of the particular guide configuration.

	Normalised Intensity (n/cm^2)		**Intensity gain over tapered collimation**		**α (°)**	**Energy integrated Intensity PRISMA**		**Energy integrated intensity ROTAX**	
	11 meV	**2 meV**	**11 meV**	**2 meV**		**(n/cm^2)**	**Gain**	**(n/cm^2)**	**Gain**
Tapered collimation (3 cm x 5 cm exit)	*0.8*	*0.2*	*1.0*	*1.0*	*0.4*	*645*	*1.0*	*10.5*	*1.0*
Tapered guide (3 cm x 5 cm exit)	6.8	3.7	8.5	18.5	2.3	5595	8.7	19.7	1.9
Tapered guide - shutter only (3 cm x 5 cm exit)	1.4	0.4	1.8	2.0	0.5	870	1.3	10.5	1.0
Tapered guide - no chopper gap (3 cm x 5 cm exit)	8.0	5.0	10.0	25.0	4.2	9285	14.4	23.7	2.3
Straight guide (2 cm x 4 cm exit)	4.4	2.3	5.5	11.3	1.5	3257	5.1	6.8	0.6
Tapered guide (2 cm x 4 cm exit)	4.5	2.5	5.6	12.5	2.0	3792	5.9	9.1	0.9

Table 1 Intensity and horizontal divergence, α, of several example beamline arrangements calculated using PRMON for the PRISMA and ROTAX sample positions. 'Tapered collimation' represents the current beamline configuration. Normalised intensity values have been calculated by dividing PRMON intensity values by the exit area of the beam.

All comparisons of intensity gains and divergence angles will be made with respect to the values for the existing tapered collimation. It can be seen from Table 1 that replacing the collimation with a guide system with an identical taper will produce a huge increase in the cold neutron intensity with factors of up to 20 above the present situation, and a correspondingly large increase at the ROTAX sample position. In fact, a factor 2 gain in intensity can be obtained just by installing a guide in the shutter section of the beamline. This increase in itself is significant, since the upgrades to the beamline will take place in separate stages during ISIS shutdown periods, leaving the instrument

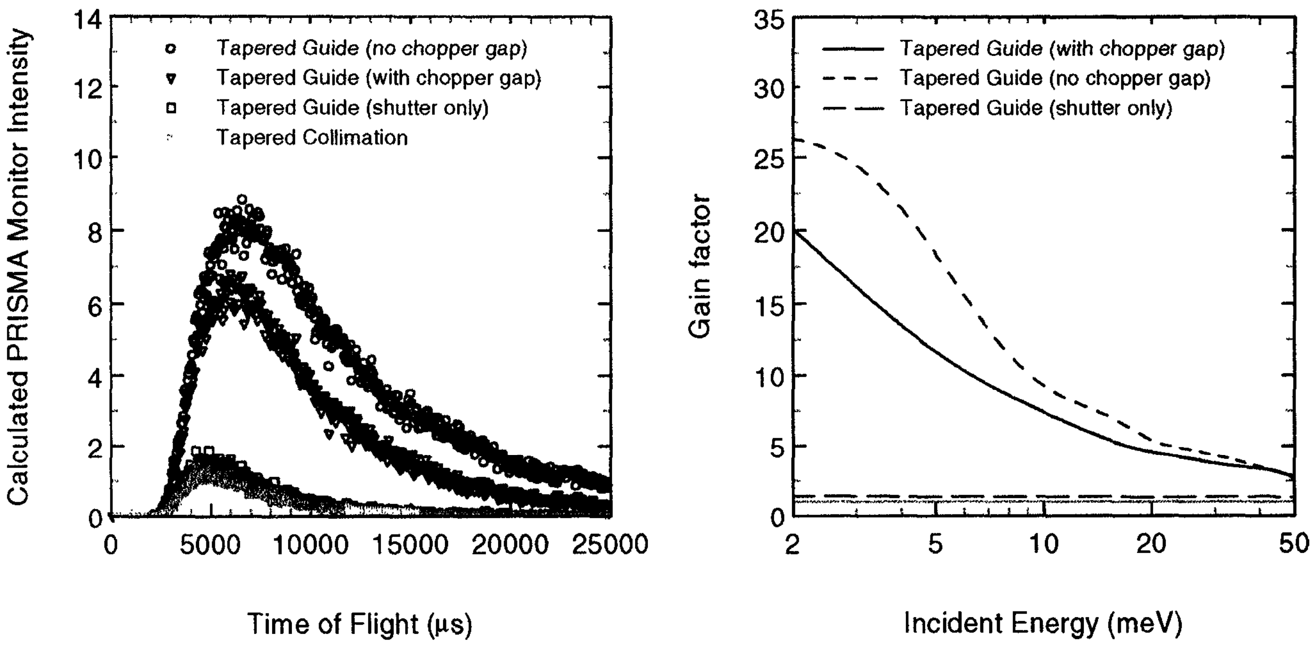

Figure 5 Calculated monitor intensities at the PRISMA sample position for the existing tapered collimation and incremental replacements of the collimation with m = 3 supermirror guide. The gain factors vs. incident energy over the present situation are also shown.

operational during experimental cycles. Consequently, users will experience the benefits of the instrument development long before the final completion date.

One of the most significant parameters affecting the transmitted intensity is the gap provided for the nimonic chopper. By replacing the gap with a section of neutron guide the intensity is enhanced by gain factors of 25 and above, but with an associated exit divergence of over 4°, principally due to neutrons with energy < 1 meV. Given that the lowest incident energy of the instrument will be 2 meV (see below), one useful feature of the chopper gap will be the removal of these unwanted neutrons. In Figure 5, the calculated monitor spectra for these three tapered guide arrangements are shown and compared to that of the tapered collimation. The gain factors for each configuration are also shown.

Since most samples rarely exceed 1-2 cm^3 and the beamline is to be optimised for a high signal:noise ratio in the presence of complex sample environment, a small final beam size, e.g. 2 cm width and 4 cm height, will be required to match the incident beam to the sample size. In Table 1, the calculated intensities for a straight guide with this cross-section, and a guide with the same taper as the existing collimation are also listed, and the calculated divergences are shown in Figure 6. As expected, the tapered collimation has a triangular divergence, which is preserved for the straight guide but with a larger divergence due to the critical angle of the supermirror. The tapered guide produces a rather interesting fringe pattern, with a sequence of minima occurring at integer multiples of the guide taper angle. Whilst the reduction in cross-section still leads to large gain factors for PRISMA, there is a detrimental effect for the ROTAX sample position due to the non-optimum matching of the beam size across the PRISMA sample area. Thus, despite the restraints upon the guide geometry, it can be appreciated from the examples given here that there are still many parameters that can be adjusted to optimise the guide system, and that furthermore, the impact upon the *entire* beamline of each parameter must be considered in the design.

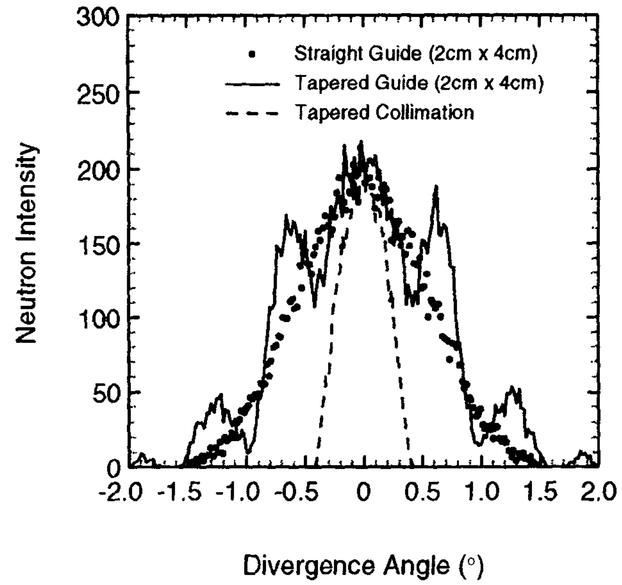

Figure 6 Calculated horizontal divergence profiles for neutron guides with 2 cm x 4 cm cross section compared with the divergence of the existing beamline collimation.

4. Optimising the beamline

The scientific case for the upgrade of the PRISMA beamline has identified three areas where the enhanced low energy flux could make a significant impact: (i) quantum critical phenomena of small moment heavy-fermion systems under pressure; (ii) lattice dynamics at high pressure, and (iii) phase transitions and dynamics of unconventional magnetic materials. All three areas will require an instrument with a high signal:noise ratio, and it is planned to install a range of devices to reduce the background of the beamline. In addition to the nimonic chopper to reduce the epithermal neutron flux, a variable aperture double disk chopper will allow the required energy window for a particular experiment to be stringently defined. Incident neutrons with $E_i > 80$ meV will also be filtered out by a removable 100 mm perfect single crystal of sapphire, and the exit beam size will be further reducable by a set of variable neutron absorbing slits. Other options will be available to allow the beam characteristics to be tailored to a particular experimental situation, including a focussing supermirror nose and Soller collimation to reduce the divergence of the exit beam.

At a spallation neutron source, tight fitting shielding around the supermirrors is critical in minimising the background from neutron and gamma radiation passing down the beam tube around the outside of the guide. Conventional guide systems are constructed from supermirror components deposited on glass substrates attached to the inside of evacuated beam tubes, but it has recently been demonstrated [6] at the ILL that m = 3 Ni/Ti supermirrors can be deposited on polished metal substrates, including steel, with equivalent reflectivity profiles to conventional supermirrors. This is a highly significant development and it is planned to construct the PRISMA neutron guide from supermirrors coated on the steel components that will be used for the insert assemblies. It is anticipated that that this will also lead to a considerable reduction in the background levels in the sample area.

The substantial increase in incident flux at low incident energies provided by the neutron guide will lead to a significant frame overlap problem. Hence, neutrons with $E_i < 2$ meV will be removed from the incident beam by a frame overlap supermirror on a glass or etched silicon substrate. The shallow critical angle will result in a length of around 1.7 m to cover the entire beam area and it will be located inside the target wall guide section where any possibility of an increased background at the sample position from the scattered beam will be minimised.

5. Summary

The development of the PRISMA instrument at ISIS into a high intensity cold neutron spectrometer optimised for single crystal experiments and extreme sample environment conditions has been described. The design phase of the supermirror neutron guide is in progress using Monte Carlo modelling techniques with completion expected within the next 6 months. Installation of the guide system will take place in stages over the next 2 years with final commissioning of the instrument during the year 2000.

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