The Powder Diffractometers

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HIPD

The high intensity instrument has been designed to provide the highest practical intensity consistent with a resolution in the range $3.10^{-3} < \Delta d/d < 10^{-2}$.

The design of the detector tank is shown in Figure 1 and a list of the instrument design parameters is given in Table 1. The principle design aims are set out below:

Moderator

Although the prime aim of HIPD is to provide a high intensity facility some thought must also be given to the effective resolution. A figure of merit

$$M(\lambda) = I(\lambda)/\Delta t(\lambda)^2$$

may be used to assess the relative performance of possible moderators. However, for powder diffraction there are two values of Δt which are of interest:

- A width (Δt at $\frac{1}{2}$ height, say) which may be used as a measure of the peak resolution.
- A width (Δt at 1/10 height, say) which may be used to determine the ability to gauge the 'background' spectrum beneath Bragg peaks.

Using $\Delta t_{\frac{1}{2}}$, the values of $M(\lambda)$ for Gd-poisoned or cooled moderators are only slightly higher than those for an unpoisoned ambient moderator. However, when $\Delta t_{1/10}$ is used the values of $M(\lambda)$ for Gd-poisoned or cooled moderators are much higher than those for an unpoisoned ambient moderator.

Detector tank

In a situation in which the detection rate is limited by the detector/data acquisition system it is imporant to eliminate extraneous background counts since each one, while adding to the statistical uncertainty, also eliminates a possible sample count. For this reason the sample tank will be evacuated and secondary collimation will be provided to reduce the detection of background counts from cryostat tails etc.

Detectors

The detectors are of the ^{6}Li glass scintillator type. The large, focussed 150° detector is the primary detector which has been optimised for intensity at good resolution ($\sim 3 \times 10^{-3} - 10^{-2}$). It is divided circumferentially into 100 x 5 cm segments. This fulfills two functions:

- The 100 detector elements and their parallel data acquisition paths permit an instantaneous count rate of 100 n/µs with only a 10% dead-time correction.
- The 2° segmentation permits anisotropic scattering to be detected.

In addition, two other detectors are provided. The 30° detector has a moderate resolution ($\sim$ 2%) and is segmented. It is provided to extend the d-range of the 150° detector.

The 10° detector has a poor resolution ($\sim$ 6%) and is not segmented. It is not intended to provide accurate data for refinement but to ensure that large d-spacing reflections are detected. A knowledge of these reflections is essential to index new patterns.

Data Acquisition

In typical diffraction patterns (eg $A\ell_2O_3$) the largest peak accounts for a few per cent of the entire diffracted intensity. Thus if total count rates of 10^6 n/s are to be maintained the system must be able to cope with $\sim$ 800 n within a particular Bragg peak (assuming ν = 50Hz). This corresponds to a peak detection rate of $\sim$ 40 n/µs. By using 100 sectors in the detector, each with its own data acquisition chain (with a $\tau_d \sim$ 100ns) the worst dead-time correction is kept down to $\sim$ 4%. For powder diffraction patterns recorded over time scales $\sim$ 20 ms it is found that a large fraction of the neutrons ($\sim$ 80%) is detected over a small fraction ($\sim$ 12%) of the total time available for detection. This means that some intermediate memory should be provided to store all events within a particular frame (ie within the 20 ms period). Currently it is envisaged that this intermediate memory will be provided in the form of 100 x 256 wd. dual-memory buffers - one for each detector segment.

The final descriptor has a maximum length of 18 bits. This may be built up from combinations of a space descriptor (n_s <8), time descriptor (n_t <13) and period descriptor (n_p <6). The latter is a tag applied to longer periods of time (ms - s) which is required in studying relaxation phenomena.

HRPD

The high resolution instrument (HRPD) has been designed to provide the highest practicable resolution consistent with reasonable counting times. Using the time-of-flight method it appears that resolutions in the region of $\Delta d/d = 3.10^{-4}$ may be reached, an improvement of a factor ~ 7 over existing high resolution neutron diffractometers. Such an improvement is important in two areas, structure determination and phase transitions.

The proposed design of the detector tank is shown in Figure 2 and a list of the main design parameters is given in Table 2. Some explanations of the choices are given below:

Guide

The guide cross-section, curvature and straight-section length have been optimised using the program MCGUIDE (1). The details of the optimisation have been given elsewhere (2). The aim of the optimisation has been to maximise the intensity of the wavelength range 0.8 - 4 Å while maintaining a uniform beam profile at the guide exit.

Disc Choppers

Disc choppers are provided at 6 m and 10 m to prevent frame overlap. Three apertures are provided to enable 1, 2 or 3 frame superposition.

Detectors

The two detector system (back scattering and low angle) are located inside the evacuated detector tank. The prime (back scattering) detector consists of 20 concentric rings lying in a plane perpendicular to the neutron beam. Time focussing is not achieved geometrically, but electronically before the event is registered. The provision of the low angle detector is for the same reason outlined in the HIPD description. It will be noticed that by having two sample positions and two detectors, four detector angles are effectively provided.

Data Acquisition

This follows the same scheme as that for the HIPD instrument. The major difference is in the larger number of time channels (32K) that must be provided.

References

[1] "MCGUIDE: A Thermal Neutron Guide Simulation Program" - M W Johnson, Rutherford Laboratory Report RL-80-065.

[2] "Neutron Guides on Pulsed Sources" - C J Carlile, M W Johnson and W G Williams, Rutherford Laboratory Report RL-79-084.

TABLE 1 HIPD parameters

MODERATOR	10 x 10 cm cooled or Gd poisoned
PRIMARY FLIGHT-PATH	9 m evacuated. Normal to moderator
PRIMARY COLLIMATION	Up to 5 x 5 cm at sample position. Collimator contains baffles to prevent multiple scattering.
DETECTOR TANK	Evacuated 10^{-1} torr for normal running (10^{-6} torr available). $\geqslant$ 20 cm boron/wax shielding.
DETECTORS	All Li glass scintillator. 150° - focussed array of 100 x 2° elements solid angle $\Omega = 0.3$ sr $L_2 = 1$ m. 30° - Unfocussed ring of 100 x 2° elements $\Omega = 0.017$ sr $L_2 = 1$ m r = 50 cm. 10° - Unfocussed ring of 1 element $\Omega = 0.005$ sr $L_2 = 87$ cm r = 15 cm
MONITORS	2 monitors at - 40 cm and + 100 cm from the sample position.
DATA ACQUISITION	150° - 100 x 256 wd (20 MHz) dual-memory buffer 30° - 25 x 256 wd (20 MHz) dual-memory buffer 10° - 1 x 256 wd (20 MHz) dual-memory buffer Overall limit of 10^{6} events/s set by memory incrementation speed. Bulk memory = 0.25 M wd ie $n_t.n_p.n_s \leqslant 0.25 \times 10^{6}$.
TIME SORTING	$n_t \leqslant 8192$ chan. Time boundaries may be software set.

TABLE 2 HRPD parameters

MODERATOR	10 x 10 mm cooled or Gd poisoned.
PRIMARY FLIGHT-PATH	100 m evacuated curved neutron guide.
GUIDE PARAMETERS	width 2.5 cm height 8.0 cm length of sections = 1 m 4 m - 6.5 m straight 6.5 m - 60 m curved: r = 18 km 60 m - 100 m straight $\lambda^* = 0.98$ Å
DISC CHOPPERS	At 6 m and 10 m. 3 apertures corresponding to 1, 2 or 3 frame supperposition. Variable speed at ν, $\nu/2$, $\nu/3$ etc.
DETECTOR TANK	Evacuated (10^{-1} torr normal, 10^{-6} available) light shielding. 2 sample positions at 1 m and 2 m from back-scattering detector.
DETECTORS	1 Back-scattering: 200 elements, 20 rings. r_{min} = 7 cm r_{max} = 37 cm.

	1 m	2 m
Ω	0.37	0.1
$2\theta_{min}$	160^o	170^o
$2\theta_{max}$	176^o	178^o

2 Low-angle:
1 element
r = 18.5 cm.

	1 m	2 m
Ω	.005	.04
2θ	7^o	20^o

MONITORS	2 monitors at - 275.5 cm and 75 cm from 2 m position.
DATA ACQUISITION	1 100 x 128 (20 MHz) dual-memory buffers 2 1 x 128 (20 MHz) dual-memory buffers Bulk memory = 0.25 M wd.
TIME SORTING	n_t < 32 K channel time boundaries s/w set.

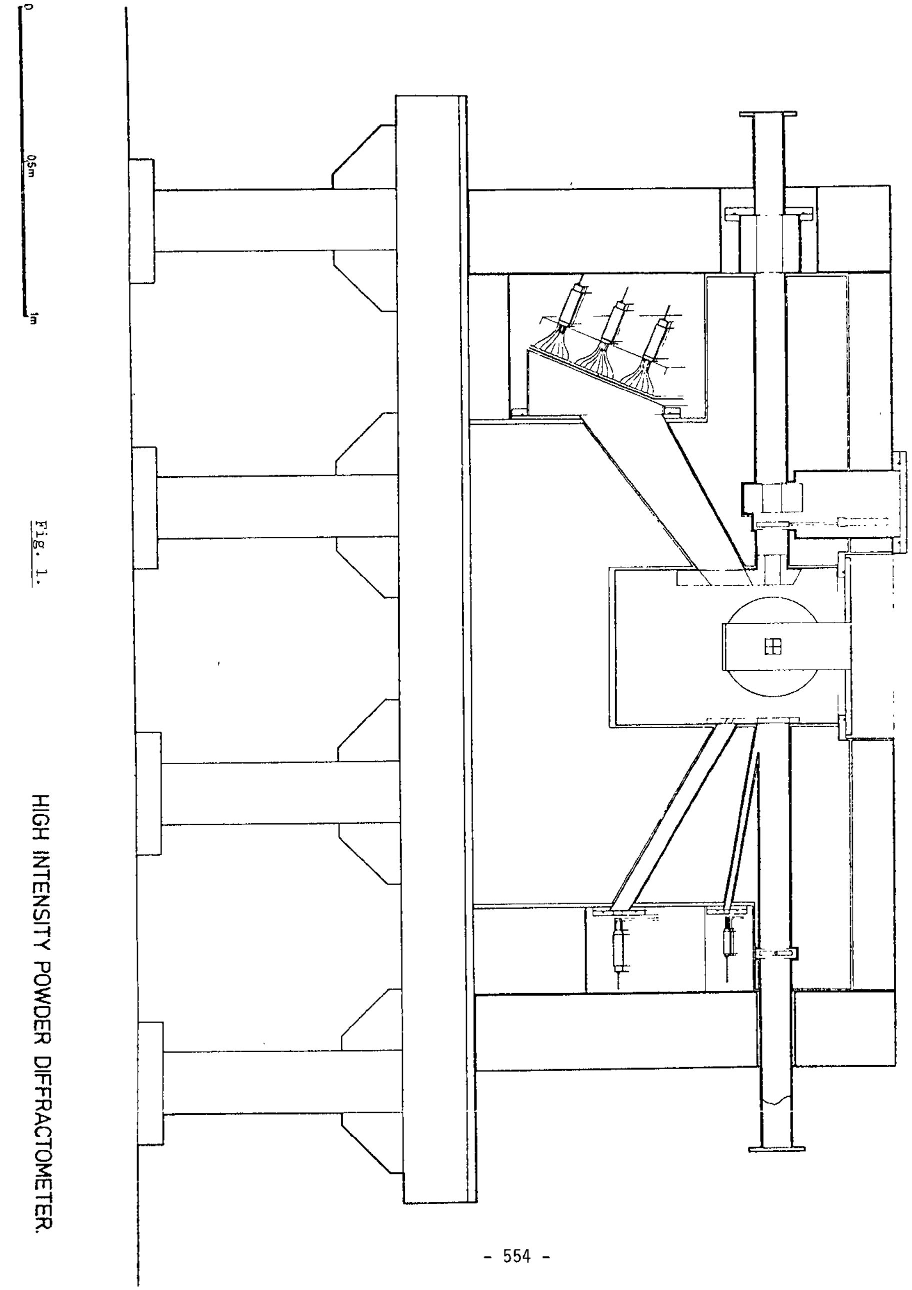

Fig. 1.

HIGH INTENSITY POWDER DIFFRACTOMETER.

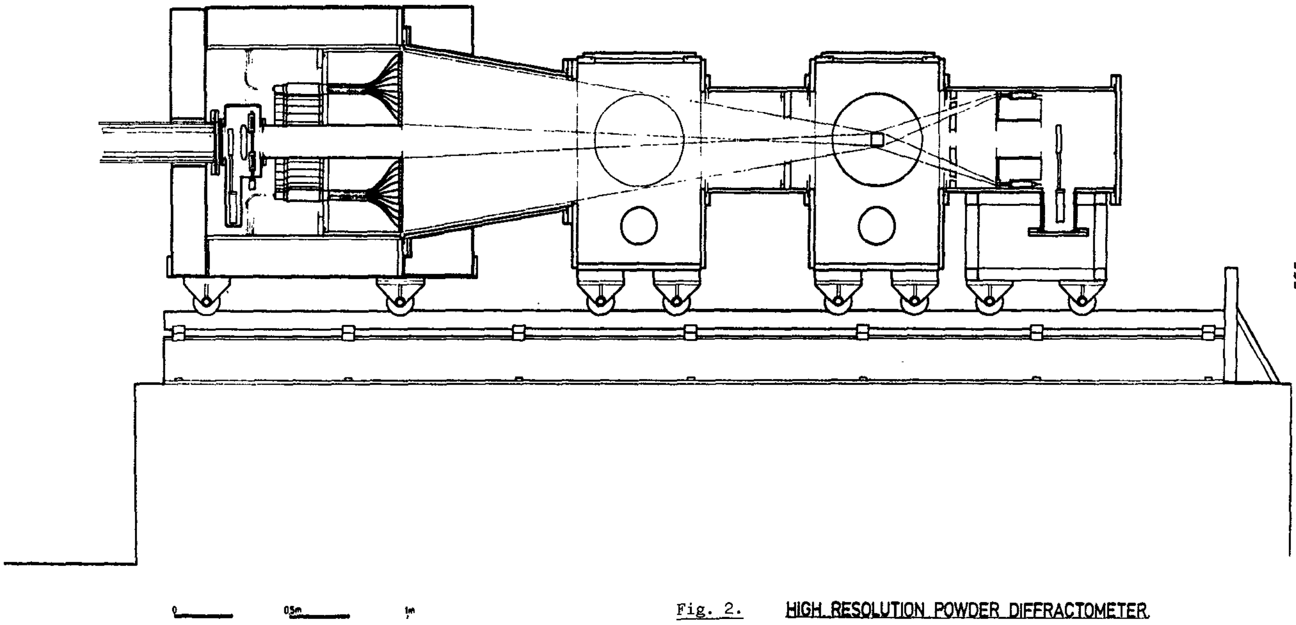

Fig. 2. HIGH RESOLUTION POWDER DIFFRACTOMETER