Proceedings of the Eighth Meeting of the International Collaboration on Advanced Neutron Sources (ICANS-VIII)
8-12 July 1985, Rutherford Appleton Laboratory Report RAL-85-110

DEVELOPMENTS IN LIQUID DIFFRACTION ON THE SNS

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1. Results from LAD on SNS

First results have just been obtained on the Liquids and Amorphous Diffractometer (LAD) on the SNS. The instrument was constructed several years ago and spent 2 years operating on the Harwell Linac before returning to RAL for installation on the SNS. A brief run was carried out in December 1984 and commissioning of the instrument started in July 1985. The instrument views the 90K liquid methane moderator and the incident spectrum as measured by the scintillator monitor is shown in figure 1 (not corrected for monitor efficiency). Small discontinuities due to the Bragg edges from the aluminium windows are just visible. Calibration will be carried out using a standard nickel powder and resonance foils. The raw nickel powder pattern for the 150° backward angle bank is shown in figure 2. The resolution has been calculated to be ~ 0.5% (standard deviation). The pattern for the lower angles (90° down to 5°) are shown in figure 3. Resolution in the short time region (around 1 eV) is better than on the Harwell Linac and this is most obvious in the low angles where the main peaks are at short times. The fast neutron background from the power pulse decays away by about 100 μs, so there are encouraging signs that energies up to 50 eV may be usable.

2. New Design for SANDALS

The original design for the SANDALS instrument was presented at the ICANS-IV meeting(1). Since then experience gained on existing pulsed sources has shown that the use of short wavelengths and low scattering angles can dramatically reduce the need for corrections for inelastic scattering. Although large scattering angle (150°) detector banks provide high count rates, interpretation of the data is often difficult. Results on silica using reactor and pulsed source instruments show that the corrections are unreliable above about 90°; for samples containing elements of lower mass the upper limit in angle could be as low as 20°. The solution is therefore to concentrate the detectors into forward scattering to reduce the inelastic correction and extend the Q range at a particular angle by using higher energy neutrons (up to 100 eV, say).

The instrument is designed for the Q range from 0.05Å^{-1} to at least 50Å^{-1}. The upper limit ensures adequate resolution in real space when Fourier Transforming the data. Maximum scattering angle is to be 50° and Q-resolution at around 30° scattering angle should be $\leq$ 1%. The sample position will be at 14m from a cold methane moderator and maximum sample size of the order 20 mm diameter. The detectors will be of Li^6 glass scintillator - a 5 mm thick scintillator has an efficiency of 30% at 10 eV and 10% at 100 eV. A schematic layout of the instrument is shown in figure 4.

3. Resolution Corrections

The effects of instrument resolution are not often considered in liquid structure calculations whether on reactor or pulsed source instruments. Problems analysing recent data taken on the Harwell Linac instruments, TSS and LAD, prompted a study of the resolution on pulsed souce diffractometers. The resolution function can be considered as the convolution of a Gaussian representing the geometrical effects and a decaying exponential to describe the source emission time distribution within the pulse. The shape of the Bragg peaks are then asymmetric and its centry of gravity is shifted from the nominal position. The effect this has on liquid structure has been investigated by calculating a hard sphere S(Q) and folding it with the resolution function to give an 'experimental' curve. The result shown in figure 5 shows that the main peak is shifted and reduced in height. In real experimental data this shows up as a decrease in peak height as the scattering angle decreases. One method of correcting for resolution uses the moments method and in a recent paper(2) it has been shown that the technique is successful.

References

1. W S Howells, Proceedings of ICANS-IV, Kens Report, II, 1981
2. W S Howells, Nucl Inst & Methods, A235, 553, (1985)

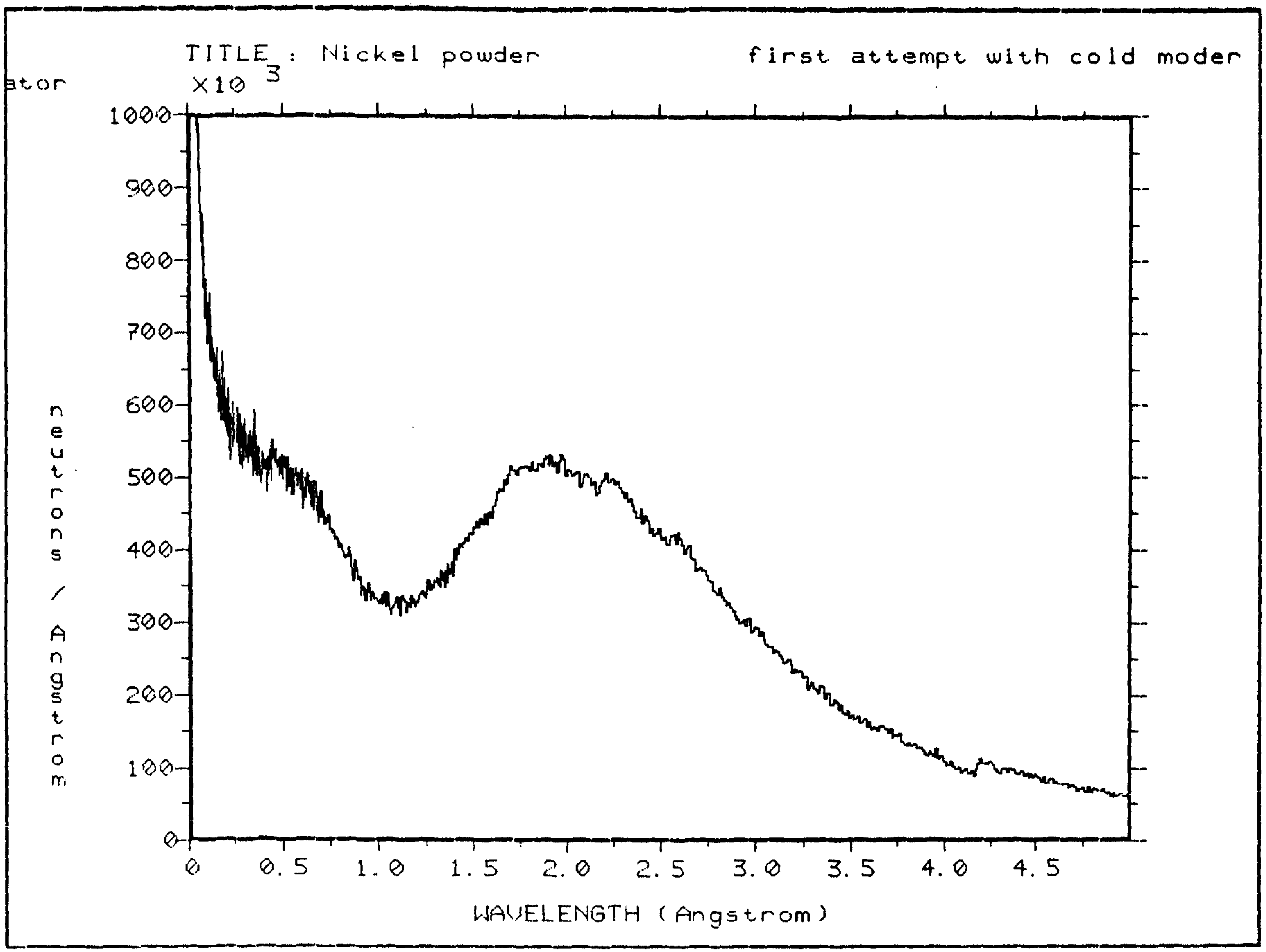
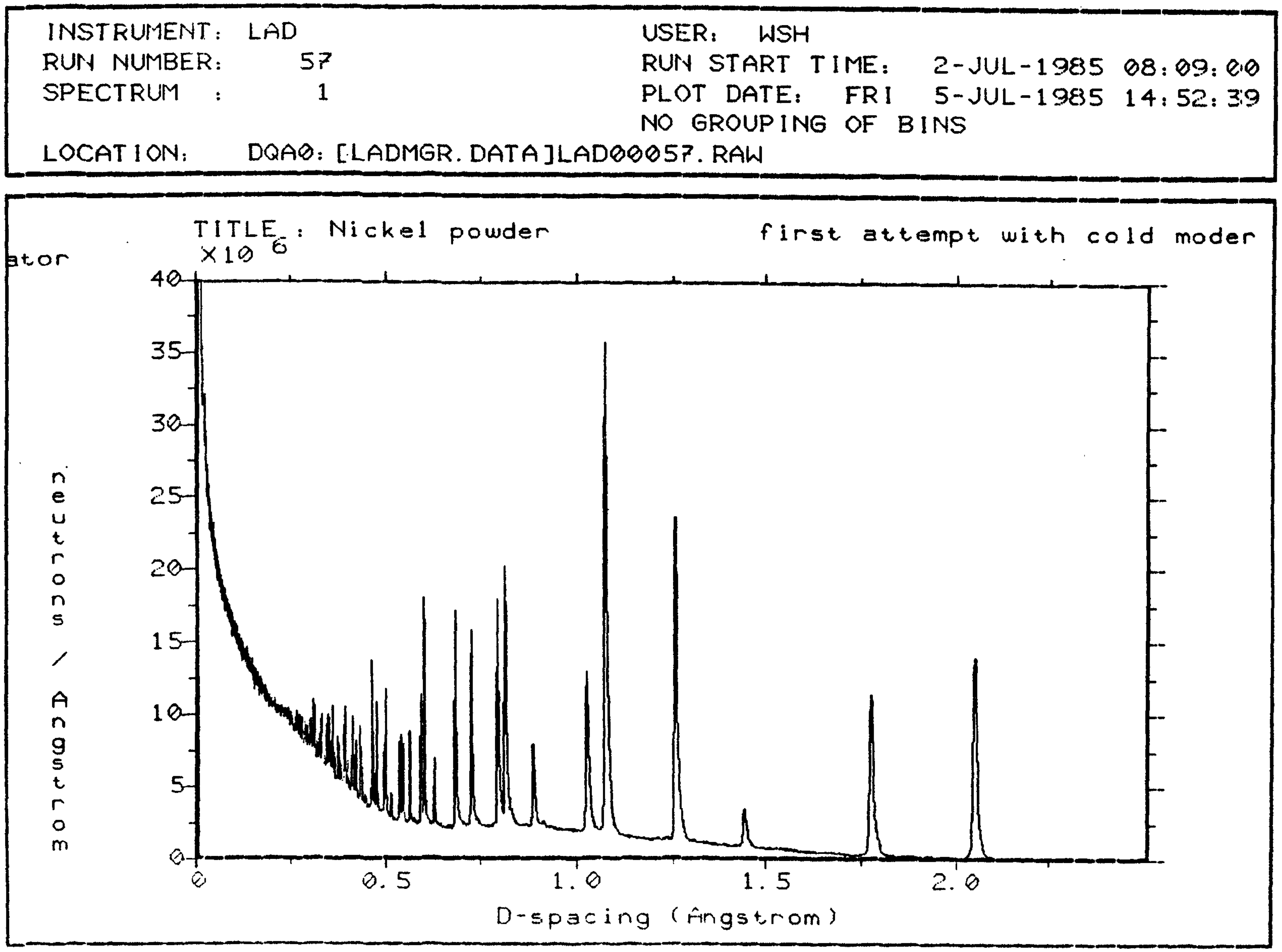

TITLE : Nickel powder first attempt with cold moder
ator
X10 3
1000
900
800
700
600
500
400
300
200
100
0
neutrons / Angstrom
0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5
WAVELENGTH (Angstrom)

FIGURE 1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RUN NUMBER: 57
SPECTRUM : 1
LOCATION: DQA0: [LADMGR.DATA]LAD00057.RAW
USER: WSH
RUN START TIME: 2-JUL-1985 08:09:00
PLOT DATE: FRI 5-JUL-1985 14:52:39
NO GROUPING OF BINS
TITLE : Nickel powder first attempt with cold moder
ator
X10 6
neutrons / Angstrom
40
35
30
25
20
15
10
5
0
0
0.5
1.0
1.5
2.0
D-spacing (Angstrom)

FIGURE 2

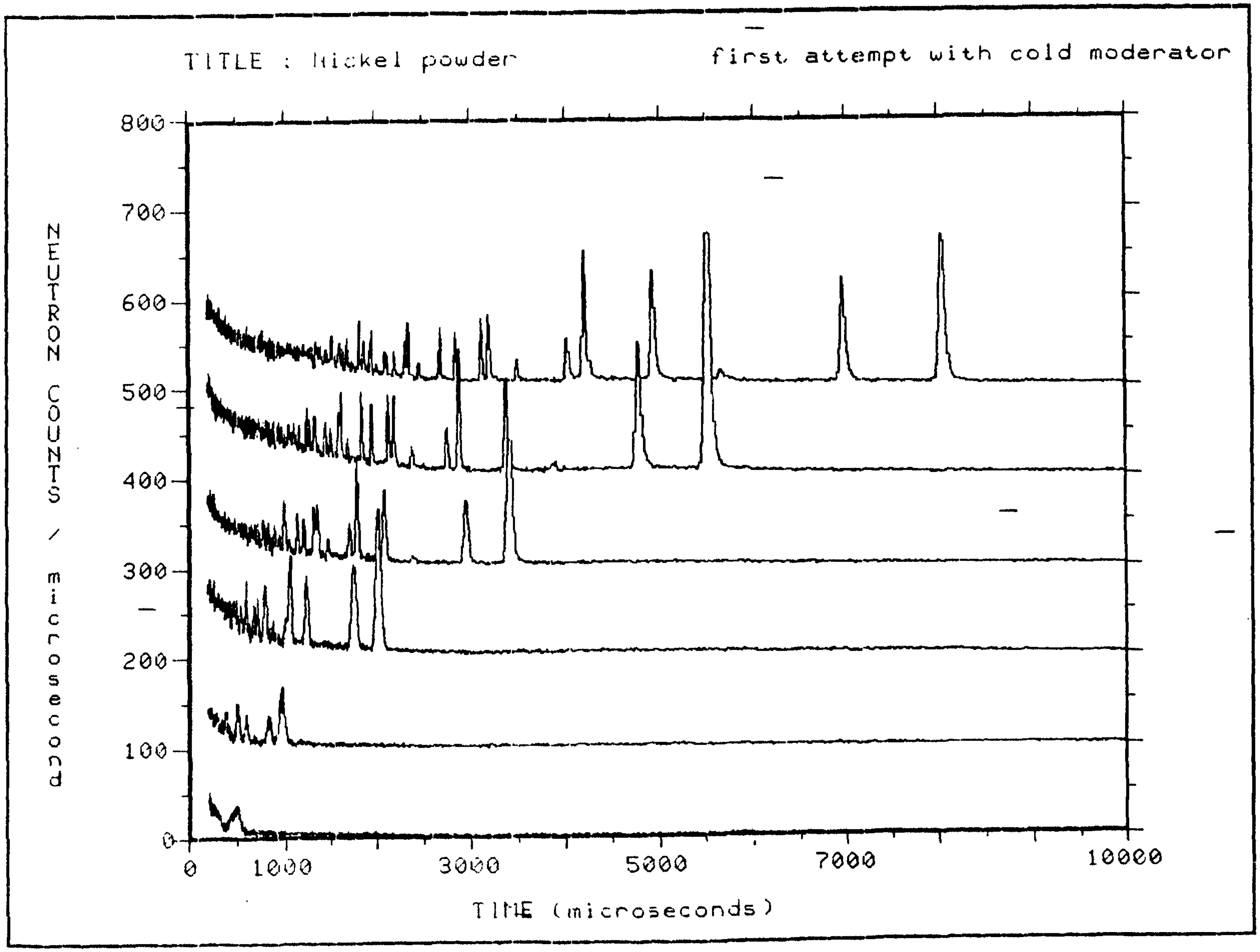
TITLE : Nickel powder
first attempt with cold moderator
NEUTRON COUNTS / microsecond
800
700
600
500
400
300
200
100
0
0
1000
3000
5000
7000
10000
TIME (microseconds)

FIGURE 3

SCHEMATIC LAYOUT OF SANDALS

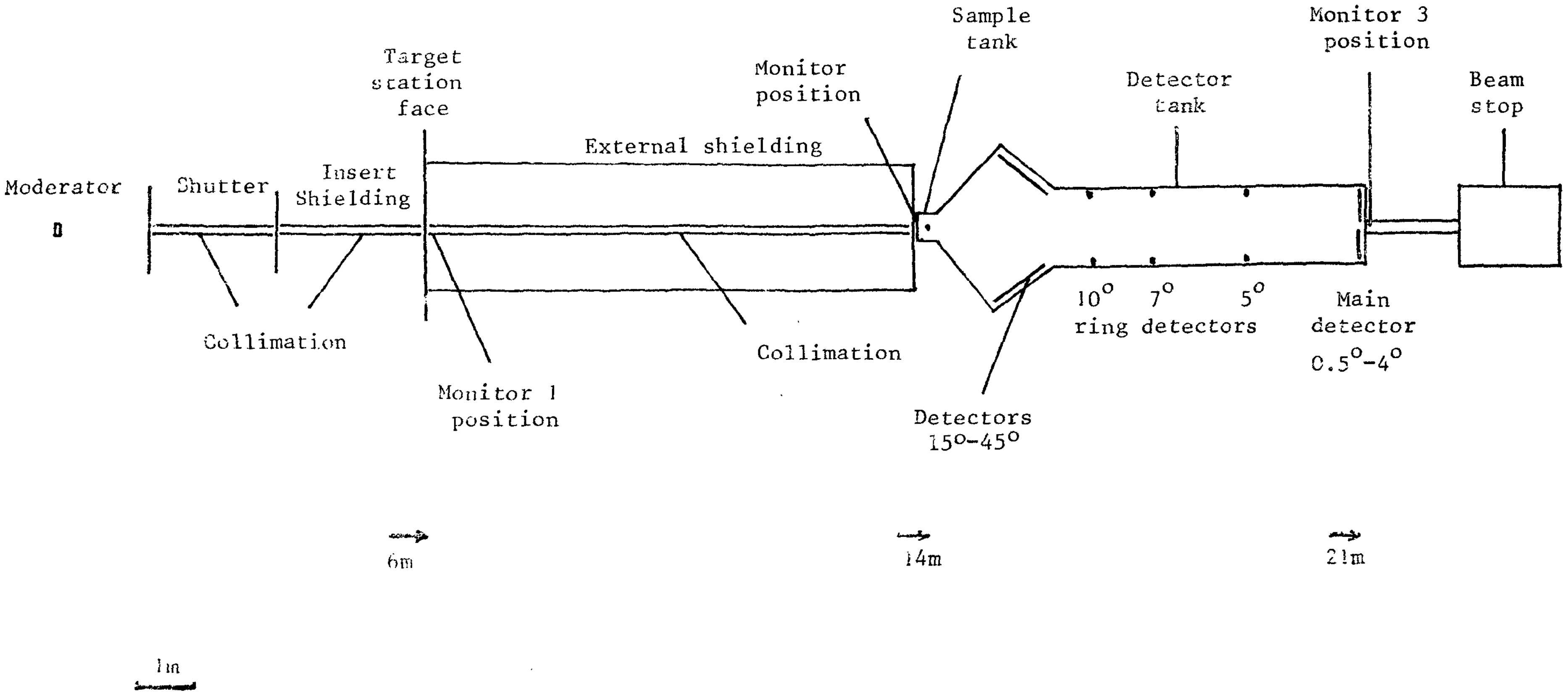

FIGURE 4

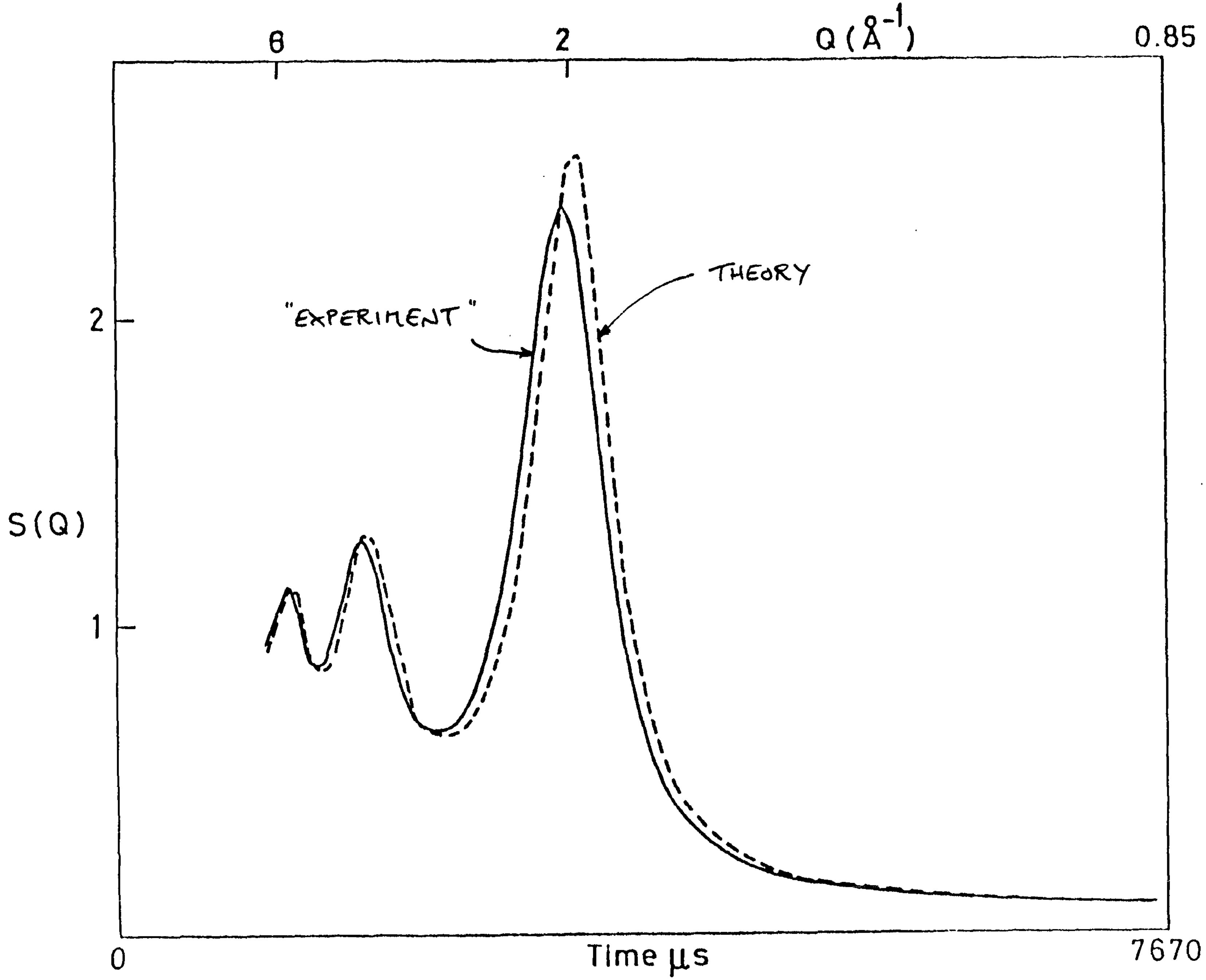

FIGURE 5