The optimisation of analyser geometry for a near back-scattering spectrometer - IRIS on the ISIS pulsed source

M. T. F. Telling & S. I. Campbell

ISIS Facility,
Rutherford Appleton Laboratory,
Chilton,
Didcot,
Oxfordshire,
OX11 OQX

June 1999

ABSTRACT

This report describes the upgrade of the pyrolytic graphite (PG) analyser bank on the IRIS high-resolution inelastic spectrometer [1] at ISIS from 1350 graphite pieces (6 rows by 225 columns) to 4212 crystal pieces (18 rows by 234 columns). The new analyser array will achieve a three-fold increase in area and in addition the graphite crystals will be cooled close to liquid helium temperature to reduce thermal diffuse scattering [2], thereby further improving the sensitivity of the spectrometer. For an instrument such as IRIS, with its analyser out of exact back-scattering geometry, optical aberration and variation in the time-of-flight of the analysed neutrons is introduced as one moves out from the horizontal scattering plane. To minimise such effects, the profile of the analyser array has been redesigned. The concept behind the design of the new analyser bank and the factors that effect the overall resolution of the instrument are discussed. Results of Monte Carlo simulations of the expected resolution and intensity of the complete instrument are presented and compared to the current instrument performance.

ACKNOWLEDGEMENTS

I. INTRODUCTION

IRIS is a time of flight (t.o.f) inverted-geometry crystal analyser spectrometer designed for high-resolution quasi-elastic and low-energy inelastic spectroscopy (Figure 1). It employs two large analysers (pyrolytic graphite and muscovite mica) oriented close to back-scattering geometry [1]. Using non-backscattering geometry avoids the loss in intensity caused by a beam modulation chopper when exact back scattering is employed.
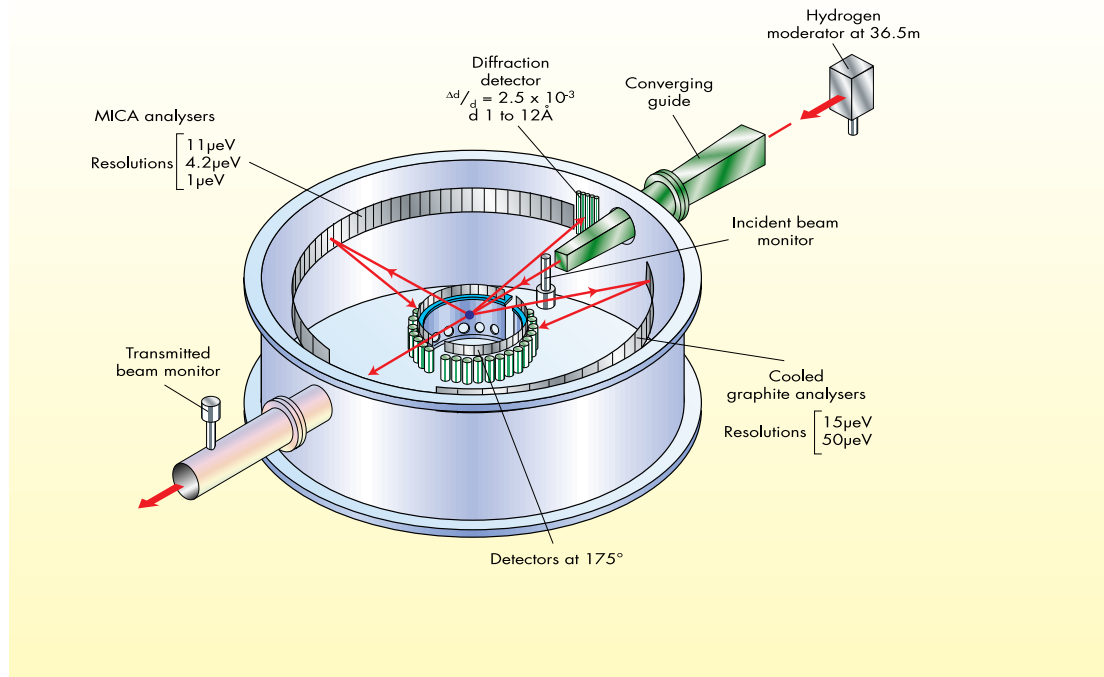

Figure 1: *The IRIS high-resolution spectrometer at the ISIS pulsed neutron source.*

The pyrolytic graphite (PG) analyser is set 0.85 meters from the sample position in the horizontal scattering plane and covers scattering angles from 15° to 165°. The present analyser consists of 1350 (6 rows by 225 columns) 2mm thick, cooled (~ 25K [2]) pyrolytic graphite pieces (10mm x 10mm) with a mosaic spread (η) of 0.8^{o} mounted on a spherically machined aluminium backing plate. The analysed beam is back scattered through 175°, slightly below the horizontal scattering plane, and detected using a multidetector composed of 51 scintillator detectors

located approximately 0.6 meters from the analyser. However, while the use of pyrolytic graphite affords the possibility of two analysing reflections, 002 and 004, with analysing energies of 1.82meV and 7.28meV and resolution of 15μeV and 50μeV respectively, the analyser itself intercepts only a small percentage (~ 1.5%) [1] of the total scattered beam. In theory, the count rate of the IRIS spectrometer may be significantly improved by simply increasing the area of the analyser.

Considering the geometric and physical constraints (shielding etc.) of the instrument, it is possible to achieve a three fold increase in the area of the graphite analyser. Such an increase equates to a new analyser array comprising of 4212 crystals (18 rows by 234 columns). While an increase in area should produce a corresponding increase in neutrons incident upon the detector, it is also important to ensure that extension of the analyser array out of the horizontal scattering plane does not degrade the current instrument resolution. Non-backscattering geometries suffer this drawback whereas backscattering geometries do not.

II. SIMULATION

Constrained by the above criteria, we have used the Monte Carlo technique to determine the optimum cross sectional profile for a new '18 row' analyser array. Simulations were performed using a graphical interface (Figure 2) calling IDL and FORTRAN subroutines [3]. The simulation procedure is shown in Figure 3.

All instrument parameters were obtained from Computer Aided Design (CAD) drawings of the IRIS spectrometer. To bench mark the Monte Carlo procedure the simulated resolution from the current IRIS '6-row' pyrolytic graphite analyser was generated. The result is compared to actual experimental data in Figure 4. The discrepancy between the two data sets at the base of the elastic line is a consequence of thermal diffuse scattering (TDS), an experimental background term highly dependant upon the temperature of the graphite pieces [2] but not yet included in the simulation procedure. While full details will be given elsewhere, it should be noted that provision has been made to cool the crystals on the new analyser to 5K. Cooling the graphite close to liquid helium temperature will further reduce background contributions arising from TDS by a factor of four over the current 25K analyser and thus significantly improve the sensitivity of the spectrometer.
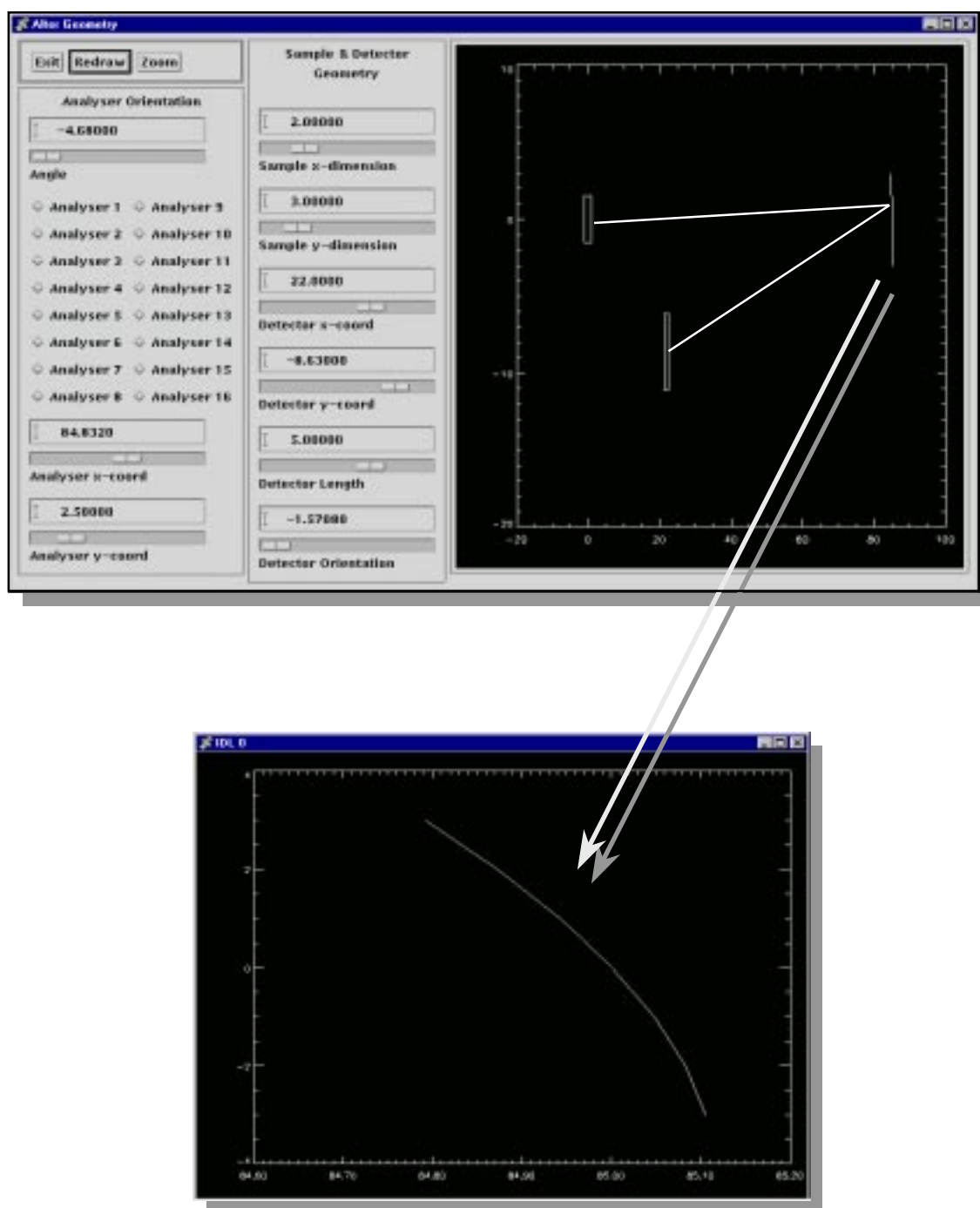
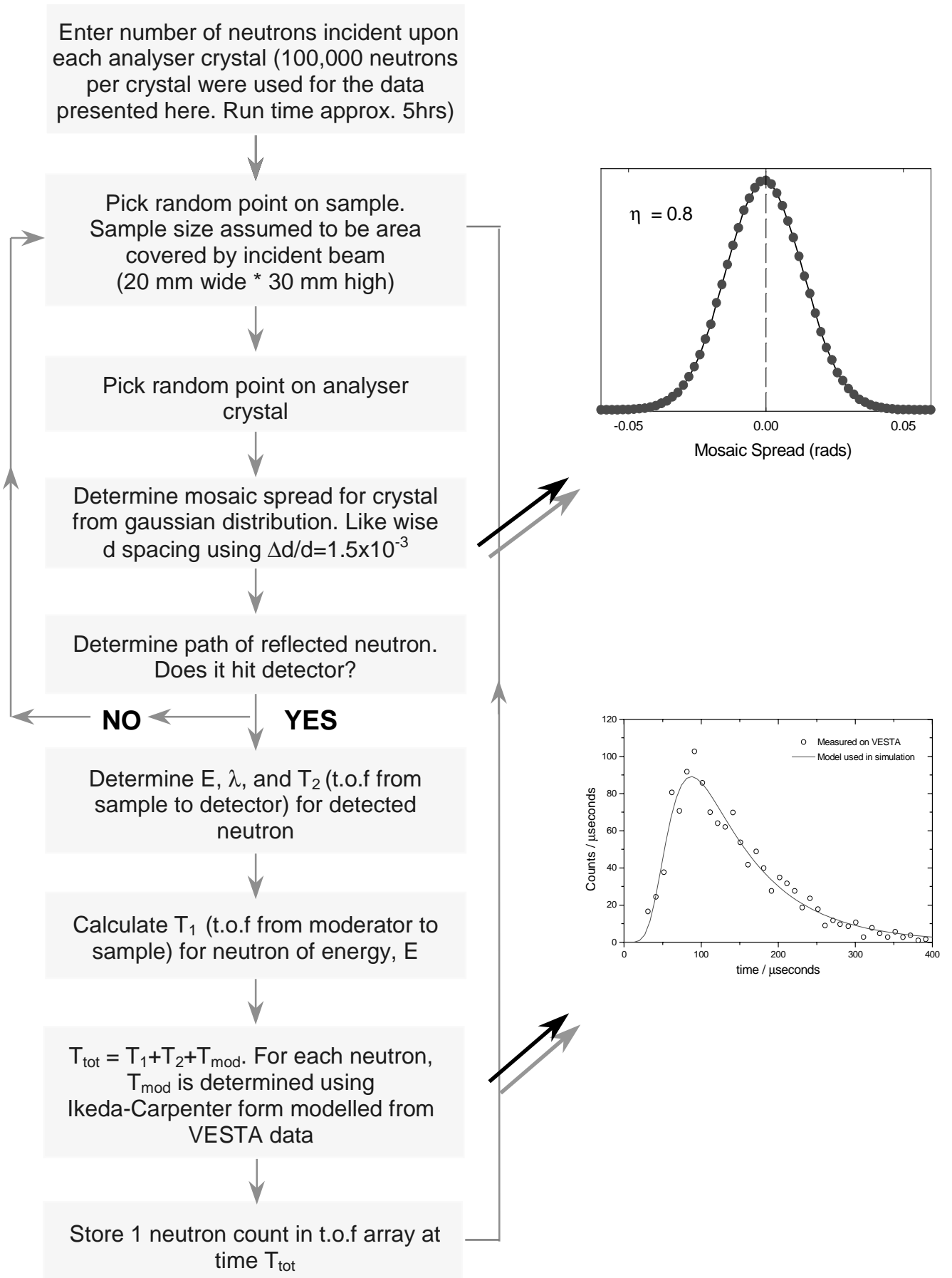**Figure 2:** *The IDL Graphical Interface*

Enter number of neutrons incident upon each analyser crystal (100,000 neutrons per crystal were used for the data presented here. Run time approx. 5hrs)

Pick random point on sample. Sample size assumed to be area covered by incident beam (20 mm wide * 30 mm high)

Pick random point on analyser crystal

Determine mosaic spread for crystal from gaussian distribution. Like wise d spacing using $\Delta d/d = 1.5 \times 10^{-3}$

Determine path of reflected neutron. Does it hit detector?

NO ← **YES**

Determine E, λ, and T_2 (t.o.f from sample to detector) for detected neutron

Calculate T_1 (t.o.f from moderator to sample) for neutron of energy, E

$T_{tot} = T_1 + T_2 + T_{mod}$. For each neutron, T_{mod} is determined using Ikeda-Carpenter form modelled from VESTA data

Store 1 neutron count in t.o.f array at time T_{tot}

$\eta = 0.8$

Mosaic Spread (rads)

-0.05   0.00   0.05

120

100

80

60

40

20

0

Counts / μseconds

○ Measured on VESTA
— Model used in simulation

time / μseconds

0   100   200   300   400
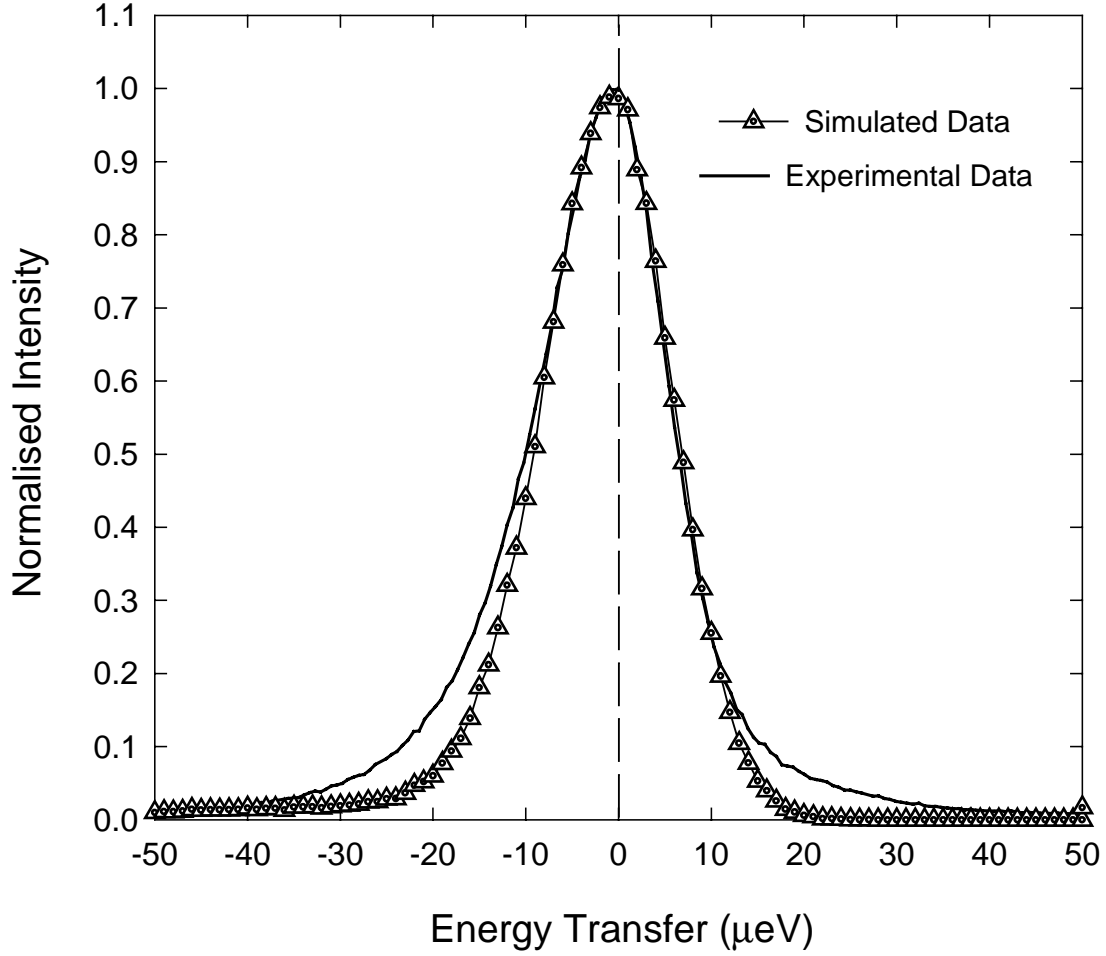
Figure 3: *The Simulation Procedure*

Figure 4: *Simulated instrument resolution from a near back-scattering spectrometer generated assuming a 6cm tall pyrolytic graphite analyser array. The data is normalised and compared to current experimental data collected from a cylindrical vanadium sample on the IRIS spectrometer. The discrepancy between the two data sets at the base of the elastic line is a consequence of thermal diffuse scattering (TDS), see text.*

III. RESULTS

The cross section profile of the current IRIS analyser was determined by considering the hybridisation of two geometrical options to i) set the analyser crystals in a near back-scattering geometry which achieves good resolution whilst obviating the need for a beam modulation chopper to increase intensity and ii) to limit optical aberration. This process hybridised the Rowland circle (constant analysed wavelength, λ_a) with an elliptical line giving a constant secondary flight path (L_2). As operation of the present set up of the spectrometer demonstrates, a

limited vertical extension of the analyser out of the horizontal scattering plane can be achieved without considerable effect upon instrument resolution. However, potentially problematic optical aberration effects worsen as this extension is increased further. Our MC calculations in fact show that for an analyser 18 crystal pieces high (i.e. 18cm high) the cross section profile favours the geometry of an ellipse. We present here two such possible profiles, A and B, with foci immediately below the sample position (Figure 5, insert 'profile A') and at the detector respectively (Figure 5, insert 'profile B').
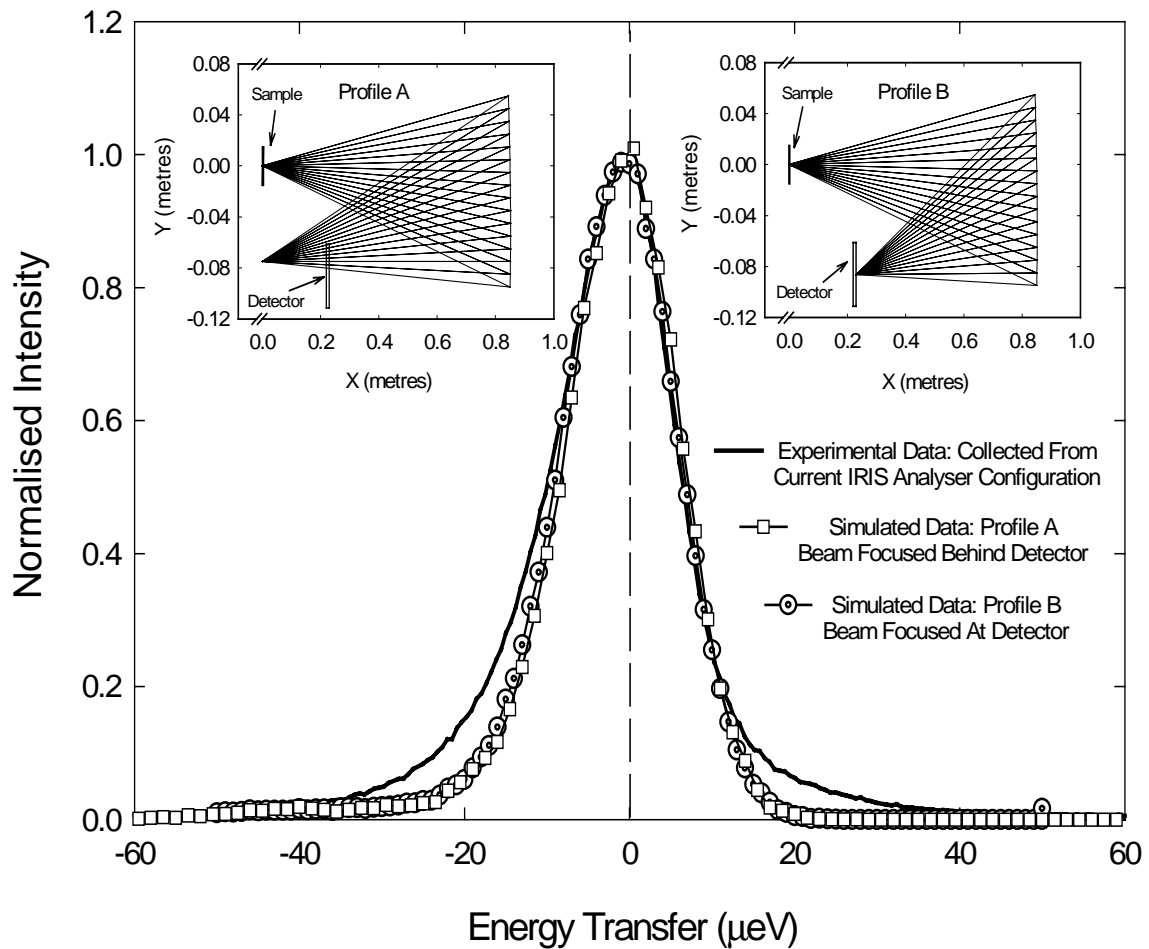

Figure 5: *Simulated instrument resolution generated assuming analyser profiles A and B. The data is normalised and compared to current experimental data. Simple ray diagrams (inserts) are presented, generated using the two different analysers crystal configurations, to demonstrate the position of the focal point of each profile.*

Considering profile A, each crystal is centred on a locus of constant path length (L_2) yet oriented such that the Bragg angle ($\theta_B=175°$) is constant. Theoretically, this configuration is most desirable since secondary flight path (L_2, sample to focus via the analyser) and analysed wavelength λ_a are constant and hence the total time of flight (t) is constant. In practice, however, neutrons reflected from the vertical extension to the analyser are not effectively intercepted by the current detector. Simulated and actual experimental spectrometer resolutions are compared in Figure 5 and the properties of the resulting analysed neutrons are detailed in Table 1. As with the current analyser array, the analysed beam converges behind the assumed detector position and the energy resolution matches that of the present analyser geometry. Of greater concern, however, considering the criteria of the analyser upgrade, is the fact that simulation suggests approximately half of all analysed neutrons in the penumbra of the beam reflected from the extended analyser would miss the present detector.

	Profile A: Focal Point Behind Detector	*Profile B: Focal Point At Detector*
FWHM of Elastic Line (μeV)	14.30 (41)	16.45 (34)
Average L_2 (m)	1.4831 (49)	1.4847 (5)
Average Analysed Energy (meV)	1.8428 (46)	1.8443 (54)
Average Analysed Wavelength (Å)	6.6628 (89)	6.6600 (119)

Table 1: *Properties of the analysed neutrons.*

The crystal configuration assumed for profile B alleviates this potential loss in detected neutrons since the detector becomes the focal point of the analysed beam (Figure 5, inset 'profile B'). However, a greater spread in λ_a is now observed since θ_B is no longer constant. The simulated resolution function is compared to that obtained from profile A, and the current instrument resolution, in Figure 5. The properties of the analysed beam are presented in Table 1 where it can be seen that the resolution is broadened by 2μeV to 16.45μeV. In addition, the neutron intensity detected for each

profile, normalised to the number of incident events, is compared in Figure 6. The integrated intensity for profile B is approximately twice that of profile A.
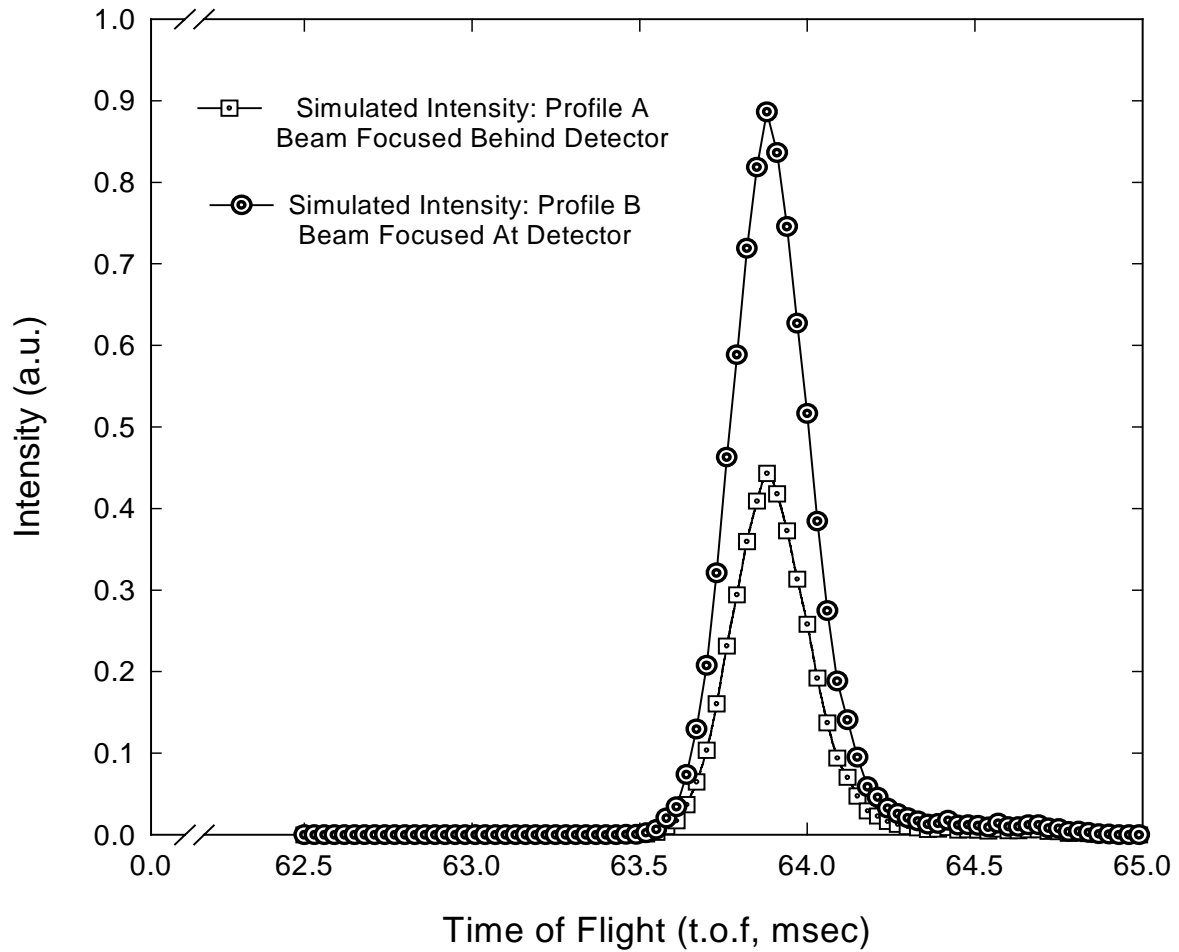

Figure 6: *Number of events detected assuming profiles 'A' and 'B'. The data has been normalised to the number of incident events used during the simulation procedure.*

A brief summary of results from Monte Carlo simulations to investigate the effect of $\Delta d/d$ and mosaic spread (η), intrinsic properties of pyrolytic graphite, upon instrument resolution is given in Appendix 1.

IV. DISCUSSION

The concept behind the design of an extended analyser bank for off-backscattering geometry has been addressed. Two profiles for the new '18 row' graphite analyser on IRIS have been suggested with expected resolution and intensity for each being simulated using Monte Carlo techniques. The results are compared to the current instrument performance.

While MC simulations of profile A suggest a slightly narrower instrument resolution, 14.30(41) μeV compared with 16.45(34) μeV for profile B, neither profile appreciably degrades current instrument resolution. In addition, both configurations exhibit a similar spread in resulting analysed neutron wavelength (λ_a) and energy (E_a). However, calculations based on profile B do highlight a two-fold increase in the number of detected neutrons. Consequently, despite the slight worsening of the resolution, we conclude that profile B represents the best over all configuration for the profile of the new pyrolytic graphite analyser on IRIS.

V. REFERENCES

1) C.J. Carlile *et al*, Physica B, 182 (1992) 431-440

2) C.J. Carlile *et al,* Nuclear Instruments and Methods In Physics Research A, 338 (1994) 78-82

3) S.I. Campbell, Ph.D Thesis, University of Salford, 1998

4) S.I. Campbell, M.T.F. Telling, C.J. Carlile (1999), submitted to Physica B

VI. APPENDIX 1

Mosaic spread, η, and Δd/d are intrinsic properties of pyrolytic graphite. The new analyser array will be constructed using graphite crystals that have a Δd/d value of 1.5x10^{-3} and a η value of 0.8°. While these values cannot be changed, it is important to understand how both limit the maximum obtainable resolution of the new analyser array, if at all. We have therefore used the Monte Carlo technique to study the effect of Δd/d and η upon the instrument resolution expected from the new '18 row' analyser array. The results are summarised below.

The breadth (FWHM) of the simulated elastic line as a function of η is presented in Figure 7. Within error, our results suggest that mosaic spread has little effect upon instrument resolution, all simulations being performed with Δd/d fixed at 1.5x10^{-3}.
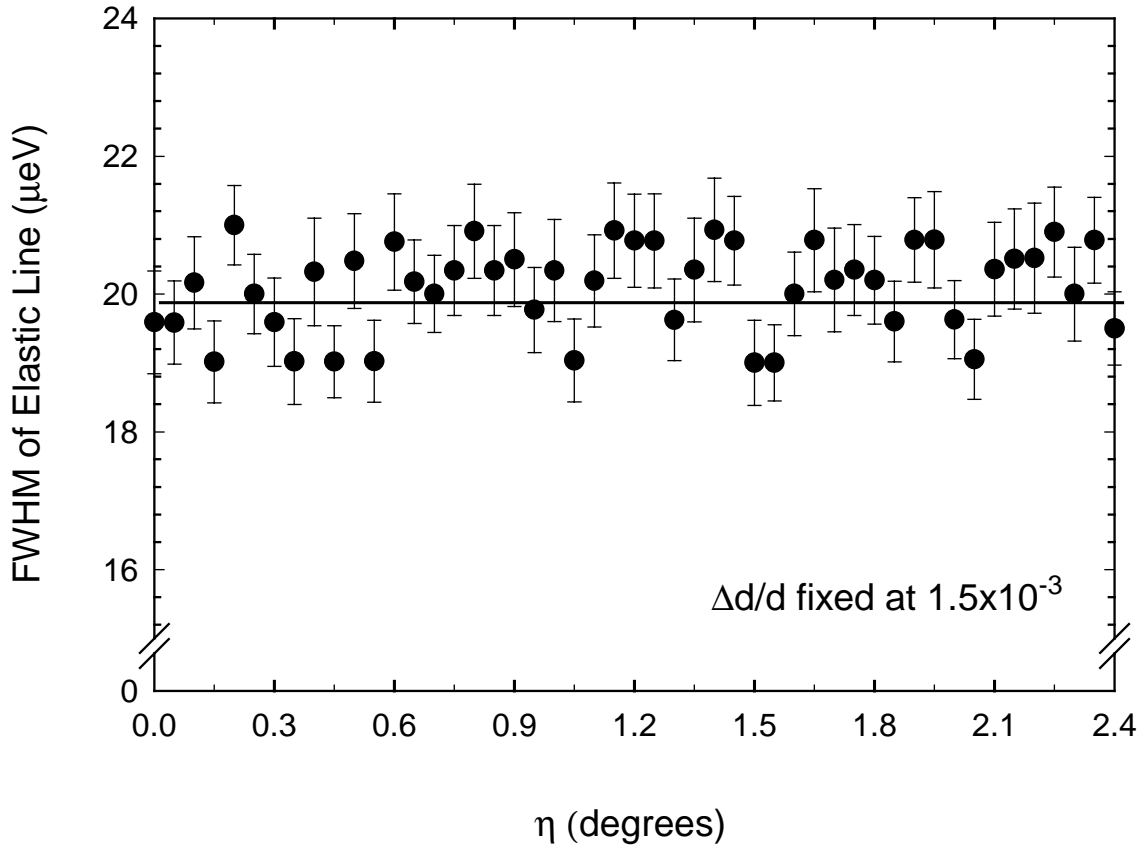

Figure 7: *The effect of mosaic spread upon instrument resolution*

In contrast, resolution is highly dependent upon $\Delta d/d$. The variation of FWHM of the elastic line as a function of $\Delta d/d$ is shown in Figure 8. We find that the resolution worsens considerably as $\Delta d/d$ is increased, the optimum value being obtained when $\Delta d/d$ is zero.
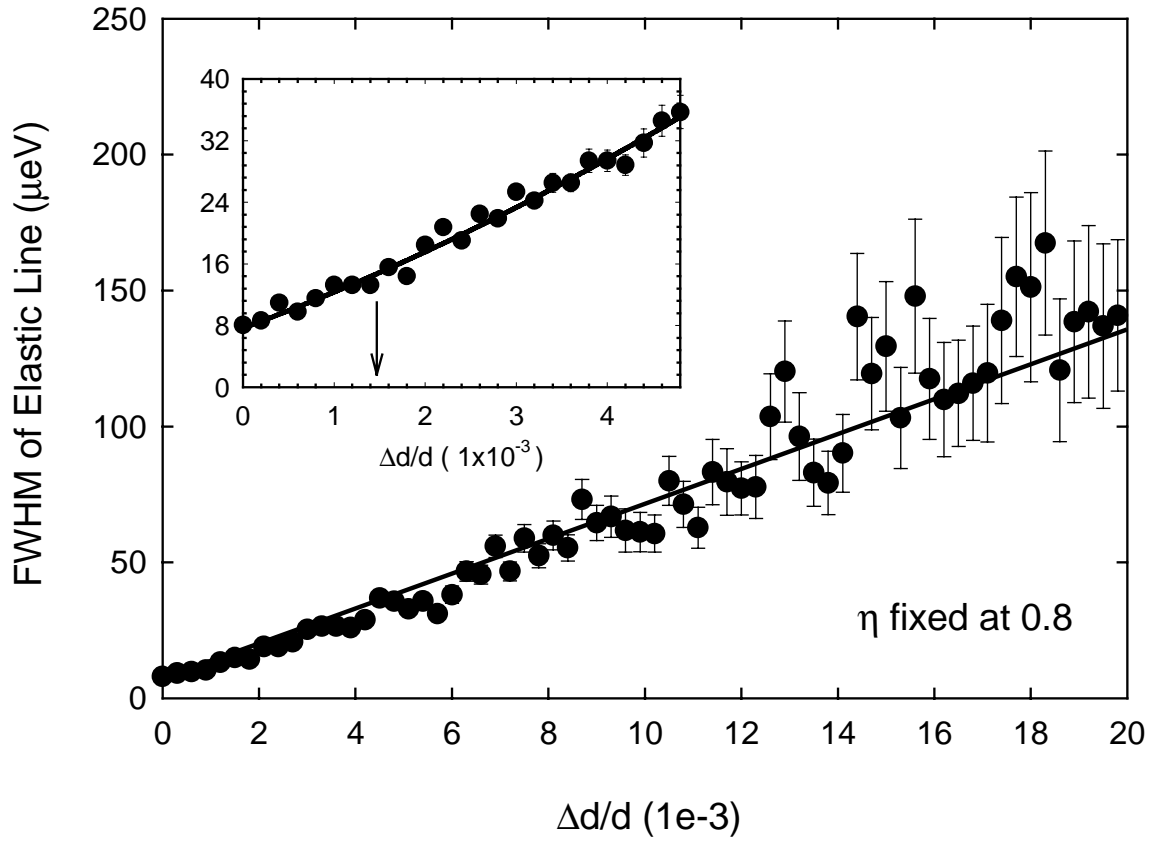

Figure 8: The *variation of the expected instrument resolution as a function of $\Delta d/d$*

Simulation suggests that for an '18 row' analyser array comprised of graphite crystals with $\Delta d/d=1.5 \times 10^{-3}$ the resolution (i.e. FWHM of the elastic line) of the instrument will never better 15μeV.