ICANS-XV
15th Meeting of the International Collaboration on Advanced Neutron Sources
November 6-9, 2000
Tsukuba, Japan

12.6 Optimisation of the design of a neutron diffractometer for strain measurement

M. R. Daymond* and M. W. Johnson
Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK
E-mail: mark.daymond@rl.ac.uk

Abstract
In this paper we describe a method for optimising the design of a time-of flight neutron diffractometer designed to measure lattice parameters. Such diffractometers are now used extensively by engineers and metallurgists for measuring strain within metallic and ceramic components. In the past neutron diffractometers have generally been built as 'all-purpose' instruments, with designs that are compromises, balancing competing requirements to measure the intensities, positions and widths of diffraction peaks simultaneously. In contrast ENGIN–X is designed with the single aim of making engineering strain measurements; essentially the accurate measurement of polycrystalline lattice parameters, at a precisely determined position. The method presented relies on the identification of a *Figure of Merit* (FOM) which accurately describes the performance of such an instrument.
Although the instrument described is based on the time-of -flight technique, the FOM derived may equally well be used to optimise a reactor based instrument. While lattice parameter measurement is a particularly straightforward example, it is shown that similar *Figures of Merit* may be found for other types of instrumentation.

1. Introduction

The general principles of neutron time-of-flight powder diffractometers has been described elsewhere [1] and in this section we simply define the nomenclature used. The essential components of a diffractometer on a pulsed neutron source are shown diagrammatically in Fig 1. Neutrons originate from the moderator (M) in short pulses (5 - 50μs) and travel to the sample (S) where they may scatter into a detector (D) situated at an angle of 2θ to the transmitted beam. The neutrons originating from the moderator have a wide energy range from a few mV up to many eV.

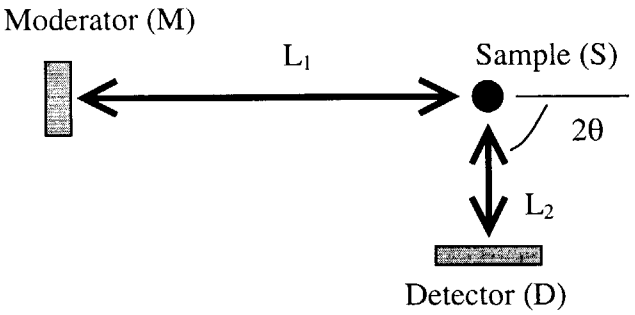

Figure 1. The main components of a time-of-flight diffractometer

While all diffractometers follow this basic layout, careful choice of instrument characteristics and optics allows the diffractometer to be tuned or optimised for particular types of experiments. The method for carrying out this optimisation for an engineering strain scanner is shown in this paper. An evaluation of the parameters required for optimisation of other types of instruments is also given.

One of the most important characteristics of a pulsed source moderator is the time-distribution of the neutron pulse, since this plays a key role in determining the resolution of the instrument. This time-distribution, typically modelled as an exponential broadened by Gaussian and Lorentzian components, may be changed by the shape of the moderator, the moderating material, its 'coupling' to the neutron source, and whether it is 'poisoned'. The shape of this pulse from the moderator controls one fundamental contribution to the resolution with which a measurement can be made.

The neutrons travel from the moderator along L_1 to the sample. A polycrystalline sample, such as most metal engineering components, will then diffract only those neutrons that satisfy Bragg's law;

$$\lambda = 2|\mathbf{d}_{hkl}|\sin\theta \qquad (1)$$

Since the wavelength λ of a neutron is related to its velocity, if the detected neutron count is plotted as a function of time (Fig. 3) it will exhibit a series of peaks corresponding to the different $\mathbf{d}_{hkl}$ lattice planes in the material. The shape of the peaks in this diffraction pattern, and hence the resolution of the diffractometer, are determined by the time distribution of the neutrons leaving the moderator and any variation in the path lengths taken by the neutrons reaching the detector. This latter contribution is known as the 'geometrical' contribution to the resolution function. Similarly, the angular contribution is defined by the moderator size as viewed from the sample, or in the case of a guide, the size of the guide aperture as viewed from the sample.

By measuring the time-of-flight (t) from the moderator to the detector, and knowing the diffraction angle (2θ) and path length L the lattice spacing d_{hkl} for the particular set of {hkl} lattice planes within the sample may be determined. Because a wide wavelength range is generally used in time-of-flight instruments a large number of diffraction peaks are recorded simultaneously, and, in the case of cubic materials, the information from all of these diffraction peaks is used to establish an average unit cell size $\boldsymbol{a}$, using the Rietveld refinement technique [2]. Having determined $\boldsymbol{a}$ it is then, in principle, straightforward to calculate the strain (ε) at that point in the sample [3]. It should be noted that the strain (ε) thus measured is a vector quantity measured along the direction bisecting the incident and scattered directions of the neutron path [3].

2. The Figure of Merit

Neutron diffractometers are generally built as 'all-purpose' instruments, and their designs are compromises which balance the competing requirements to measure the intensities, positions and widths of diffraction peaks simultaneously. In the case of an optimally designed engineering strain scanner such compromises are not necessary, since the overriding requirement of the instrument is the accurate measurement of a lattice parameter, d_{hkl}, at a known location within the material under study.

To enable different instruments to be compared it is reasonable to define a FOM such that an increase of a factor of two in the source illuminating an instrument results in a factor of two increase in the FOM. It is also necessary to take into account the uncertainty of the result obtained. Hence the most useful high-level definition of a FOM for a strain measuring instrument will be *'the inverse of the time taken to measure a d-spacing to a given uncertainty'*.

d-spacings are obtained from the observed diffraction patterns by a 'least-squares' fitting procedure, and it has been shown by Sivia [4] that in the situation of an isolated Gaussian peak the time (t) taken to measure (with an uncertainty of σ) the position of a peak is:

$$t \propto w^2 / I\sigma^2 \qquad (2)$$

where w is the width of the peak, and I the (integrated) intensity within the peak recorded in unit time. Hence the FOM required for an instrument concerned solely with measuring the peak position may be written :

$$FOM = I\sigma^2/w^2 \qquad (3)$$

if the peaks were Gaussian in shape and well separated. Although the result of equation 2 has been known for a Gaussian shape its applicability when an *arbitrary* peak shape is fitted by the least squares method is derived elsewhere [7].

Thus equation 3 may be used quite generally for establishing the performance of an instrument designed to measure the position of isolated peaks. The veracity of this result has also been demonstrated empirically [5]. This was done by deriving the position of a large number of experimentally measured peaks by least squares fitting. These were measured at different facilities (reactor and pulsed neutron sources, and an x-ray synchrotron source) on different materials.

From this it is clear that the above FOM (equation 3) must be maximised in the design of an optimised strain scanning instrument, and that the ratio of the FOM to other instruments quantifies its increased speed of measurement.

3. Maximising the flux of neutrons - solid angle and use of guides

One way in which the FOM can be maximised is by utilising the fact that the primary measuring position in a strain scanning instrument is at a scattering angle of (2θ=) 90°. At this scattering angle the widths (w) of the peaks in the diffraction pattern (and hence FOM) are insensitive to changes in the vertical angle of incidence of the incident beam [6]. Thus, while Liouville's theorem dictates that we cannot increase the flux of neutrons per unit solid angle incident on the sample (over that emanating from the moderator), we can increase the *total flux* of neutrons usefully incident on the sample by increasing the vertical divergence of the beam incident on the sample. In an optimised strain scanning instrument the vertical divergence of the neutron beam would therefore be increased to the maximum that can be achieved by the use of super-mirror guides above and below the incident beam.

However, the length of the primary flight path, and the angular divergence of the neutron beam in the horizontal plane play dominant roles in defining the widths of the diffraction peaks (w). This angular contribution must be added to the various resolution contributions

discussed above. In fact to match the horizontal angular divergence to that due to the flight path, we find that for a 50m flight path this should be set to 100/50,000. In this case the required divergence could be achieved by foreshortening the side walls of the neutron guide, such they end at a distance of 38m, i.e. 12m from the sample.
Thus we have a scenario where the intensity is increased using guide surfaces above and below the sample, but that the guide is limited in the horizontal plane in order to maintain a high resolution.

4. Optimising other instruments

It is also possible to quantify the FOM even in the presence of a substantial background, and in this case the expression becomes:

$$FOM_{\text{peak position}} = \frac{I}{w^2\left(1+2\sqrt{2}\frac{B}{P}\right)} \tag{4}$$

where P/B is the peak/background ratio.
This simple analytical result follows the method of [4] and is correct in the asymptotic cases of high background (i.e. approximately equal errors for all points) and low background (i.e. approximately Poisson statistics). In the intermediate regime, Sivia [4] suggests that the form is correct to within ~10%.

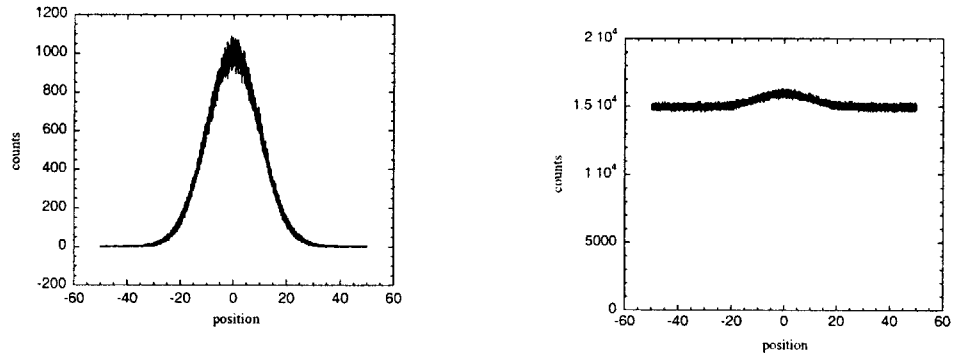

Figure 2. Simulated data, showing peaks in the case of (a) low and (b) high backgrounds. In the first case, the uncertainty for the intensity at given point within the peak changes drastically across the peak (following Poisson type statistics). In the second case, the same peak is shown on a large background. Now the high background means that the uncertainty is approximately constant throughout the data set.

The expressions for the FOM when measuring amplitude and width can also be derived following similar methods:

$$FOM_{\text{amplitude}} = \frac{I}{\left(1+\sqrt{2}\frac{B}{P}\right)} \tag{5}$$

$$FOM_{\text{width}} = \frac{I}{w^2\left(1+4\sqrt{2}\frac{B}{P}\right)}$$

The expressions in equations 4 and 5 have been analytically derived for a Gaussian peak shape, and the exact parameters in front of the B/P term may well be dependent on the actual

peak shape. It may be noted that, when B/P is high, the intensity becomes relatively more important due to the fact that P is proportional to I / *w*.

Acknowledgements

The authors would like to acknowledge Devinder Sivia for helpful discussions. The ENGIN-X diffractometer is under construction at the ISIS pulsed neutron facility at RAL under EPSRC grant GR/M51963 awarded to The Open University, Manchester University, Imperial College, Salford University and ISIS.

References

[1] C. G. Windsor, *Pulsed neutron scattering* (Taylor and Francis, London, 1981).
[2] M. R. Daymond, M. A. M. Bourke, R. B. Von Dreele, B. Clausen, and T. Lorentzen, J. Appl. Phys. **82,** 1554-1562 (1997).
[3] I. C. Noyan and J. B. Cohen, *Residual Stress - Measurement by Diffraction and Interpretation* (Springer-Verlag, New York, 1987).
[4] D. S. Sivia, *Data Analysis - A Bayesian Tutorial* (Oxford University Press, 1996).
[5] L. Edwards, M. E. Fitzpatrick, M. R. Daymond, M. W. Johnson, G. A. Webster, N. P. O'Dowd, P. J. Webster, and P. J. Withers, *ENGIN-X: A Neutron Stress Diffractometer for the 21st Century* in Proc. of ICRS-VI, Oxford, 2000.
[6] M. W. Johnson, L. Edwards, and P. J. Withers, Physica B: Condensed Matter **234-236,** 1141-1143 (1997).
[7] M.W. Johnson and M.R. Daymond, *to be published.*