

ESS Engineering Group Report

Mark R. Daymond (ISIS), Philip J. Withers (Manchester), Eberhard Lehmann (PSI)

Executive Summary

The Engineering Group strongly endorses the 50Hz SP Target. Some applications of both the 10Hz SP and 16Hz LP targets can be foreseen.

The Engineering Group would primarily make use of high resolution moderators (decoupled / poisoned). It was felt that neither the H₂ or H₂O moderator options fully met the needs of an engineering diffractometer, and that the possibility of obtaining higher resolutions using methane or hybrid moderators should be investigated.

Strain Measurement

In the case of an optimally designed engineering strain scanner 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 [1] 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:

$$t \propto w^2 / I\sigma^2 \quad 1$$

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 :

$$\text{FOM} = I\sigma^2 / w^2 \quad 2$$

if the peaks were Gaussian in shape and well separated. The correctness of equation 2 when an *arbitrary* peak shape is fitted by the least squares method is derived in [2]. The veracity of this result has also been demonstrated empirically, using experimental data from a number of sources and on a number of different materials [3].

Using this approach, the optimum design for a strain measurement diffractometer is a medium resolution diffractometer with flight path 30-50m [2]. While such an instrument might feasibly be built on the 10Hz ISIS TS-2 target, it would lose some flexibility in operating modes. Without the gains in moderator performance possible on the low power ISIS TS-2, the equivalent ESS 10Hz SP TS is not an option. There also does not appear to be a strong case for moving such an instrument the 16Hz LP TS.

On the preferred option of the 50Hz target, the Engineering diffractometer would require a high resolution moderator (decoupled / poisoned). It was felt that neither the H₂ or H₂O moderator options fully met the needs of an engineering diffractometer, and that the possibility of obtaining higher resolutions using methane or hybrid moderators should be investigated.

Radiography/Tomography

The primary requirement for traditional radiography is for high thermal or cold neutron flux, with a reasonably parallel beam. In this case, either of the 5MW targets would probably be appropriate, using an intensity optimized moderator. However, there is a large potential advantage for doing radiography on the 50Hz target, namely of carrying out Bragg edge discrimination during radiography measurements, allowing simultaneous identification of the material present. Proof of concept has been carried out at Los Alamos. At present it is a laborious process since it cannot be done electronically to a useful resolution. This is a clear detector development requirement.

To allow Bragg edge discrimination in complex materials, a moderately high resolution will still be required – the decoupled hydrogen moderator would probably be a good choice. The instrument would be a short flight path combined with collimators, to allow both a large wavelength band with the highly parallel beam required for high spatial resolution.

References

1. D. S. Sivia, *Data Analysis - A Bayesian Tutorial* (Oxford University Press, 1996).
2. M.W. Johnson, and M.R. Daymond, *An Optimum Design for a Neutron Diffractometer for Measuring Engineering Stresses*, in preparation
3. 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, in *Proc. of ICRS-VI*, Oxford, 2000.