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Optimizing constant wavelength neutron powder diffractometers

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ABSTRACT

This article describes an analytic method to optimize constant wavelength neutron powder diffractometers. It recasts the accepted mathematical description of resolution and intensity in terms of new variables and includes terms for vertical divergence, wavelength and some sample scattering effects. An undetermined multiplier method is applied to the revised equations to minimize the RMS value of resolution width at constant intensity and fixed wavelength. A new understanding of primary spectrometer transmission (presented elsewhere) can then be applied to choose beam elements to deliver an optimum instrument. Numerical methods can then be applied to choose the best wavelength.

1. Introduction

This article describes a method to analytically optimize conventional constant wavelength (CW) neutron powder diffractometers (PD). Clearly, such an optimization has academic interest. If it delivers significant performance improvements, then it also has practical interest. If it indicates the approach needed to optimize and improve other instrument types that would be a further benefit. Regardless of any potential performance improvements, such an optimization should help in better planning and running research facilities. The optimization process described here is a little complex and involves synthesizing many elements. Some approximations and simplifications are needed. An important related question, whether time-of-flight (TOF) PDs are better than CW PDs, is not addressed here since there is not yet a full optimization for TOF PDs.

The optimizations for some simple types of neutron scattering instruments are already known. If two collimators are rocked in a beam, the maximum transmission for a given peak width in the scan requires that the two collimators have equal angular width. If the widths are mismatched, the smaller restricts transmission while the larger limits resolution. If the collimators have a rectangular variation of transmission with angular divergence, $\tau(\gamma)$, the integrated transmission is a factor of 2 higher than that for triangular profiles for a given scan angular full width at half maximum (FWHM). In this case there is no contribution of wavelength spread to resolution so the wavelength spread, $\Delta\lambda/\lambda$, should be as large as possible. The optimization for pinhole type small angle neutron scattering diffractometers (SANS) [1] shows that the primary and secondary spectrometers should have equal angular divergence in two dimensions (2D) to maximize count rate for a given resolution and equal lengths (to maximize sample area). Wavelength spread here introduces angular broadening in scattering features. The optimum fractional wavelength spread for a SANS is $\Delta\lambda/\lambda \approx \Delta\theta_S \cot\theta_S$ (where θ_S is the scattering angle at the sample); this value depends on the scattered wave-vector. This optimal wavelength spread is usually surprisingly large ($\approx 10\%$). Ref. [1] states that the intensity is proportional to the fourth power of resolution width although this ignores the contribution of wavelength spread to intensity. Extensive analytic studies have developed expressions for the resolution and intensity of most important neutron scattering instrument types. However, finding the optimum for instruments more complicated than SANS using these results has proved difficult. By the end of this article, it should be clear that the optimization for CW PDs also involves matching the resolution contributions due to the allowed in- and out-of-plane angular spread before and after the sample and the resolution effect of wavelength spread. That strongly suggests that this is the general approach needed in optimizing neutron scattering instruments.

The difficulty of using the existing resolution equations to improve instruments has encouraged the use of Monte Carlo (MC) computer simulations using programs such as McStas [2] to seek instrument improvements. The usual method adopted is to choose some instrument configuration and compare its simulated performance to that of slightly different configurations. More recently, these instrument simulation programs have been used as the kernel of numerical optimization routines. The parameter space for these simulations is very large and there are usually correlations between the effects of a number of the parameters. This process would be more effective if there was some guidance as to

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which instrument configurations to simulate. Ideally, the process would also apply a quantitative quality factor but there is little guidance as to what form that quality factor should take. Therefore, most discussion of improving instruments concentrates on increasing the beam flux at the sample position and increasing the detector solid angle coverage.

An instrument quality factor describes a cost benefit trade-off. It is widely appreciated that there is an intensity-resolution trade-off on neutron scattering instruments. However, the exact form of this trade-off for each instrument type does not seem to be generally known. PDs are mainly used to determine crystal structures and their use is intimately associated with Rietveld structure refinements. It has been suggested that an optimized CWPD would be one which returned the smallest *R* value for a Rietveld analysis of a structure. The analysis of instrument resolution and intensity used in the optimization process described here suggests some elements of the CWPD quality factor. The initial view adopted here is simply that an optimized instrument would resolve peaks from each other and from background as fast as possible within the constraint of measuring some desired range of d_S, the sample crystal plane spacing. There is no question that modern CW PDs are generally far more powerful than older machines. There must be some limit to the performance possible for the broad layout used which only a full optimization can disclose. Other instrument configurations (such as TOF PDs, for example) may be found to be superior to a conventional CW PD but only by comparing optimized examples of each type can valid comparisons be made.

An earlier attempt to solve the CW PD optimization problem [3–5] deduced an expression for a quality factor, Q_{PD}, as the instrument transmission, τ, divided by the resolution to the 4th power with the resolution expressed in terms of (U,V,W) (see Eq. (1a)). Numerical methods were used to maximize Q_{PD} but the convergence was poor. It is now clear that this poor convergence was due to a poor choice of variables. Embarrassingly, that work was later found to have an error in the calculation of the resolution effect of vertical divergence where an 8ln2 term was omitted. The effect of wavelength was also ill described in that work. A corrected set of formulae was later deduced and McStas simulations of CWPD configurations optimized using those corrected formulae showed large performance improvements.

This article presents a fully analytic CW PD optimization. A recent study of primary spectrometer transmission [6], shows a path to even larger performance improvements.

2. Instrument description

The instrument considered is illustrated schematically in Fig. 1. This work assumes a horizontal scattering plane. The source (usually a nuclear reactor) is followed by a primary spectrometer (PS) consisting of some collimator of angular FWHM α_1, a crystal monochromator of mosaic β and a second collimator, α_2. The collimators may be Soller collimators, guide tubes, radial Soller collimators or open beam tubes (slit pairs). The monochromator is oriented at Bragg angle θ_M, and may be curved in the scattering plane (with radius R_{MH} - this is usually called a horizontally focussed monochromator or HFM). Vertical (out-of-plane) beam divergence is allowed. Large vertical beam divergence before the sample, $\pm\phi_2$, can increase count rates at a relatively small in-plane resolution cost. Therefore, the monochromator, of height $2H_M$, is usually curved in the vertical plane to "focus" the beam to the sample. The PS beam is scattered by a powder sample. The principal features in the scattering are usually a number of distinct Bragg peaks. Conceptually, a single detector following a collimator, α_3, is scanned through the scattering angles, $2\theta_S$, to produce a plot of scattered count rate as a function of angle. It is usual practice to use multiple detectors or a continuous position sensitive "banana" detector (PSD) to increase the count rate. The detector height, $2H_D$, is usually much larger than that of the sample, $2H_S$. This increases vertical divergence after the sample, $\pm\phi_3$, and hence the count rate.

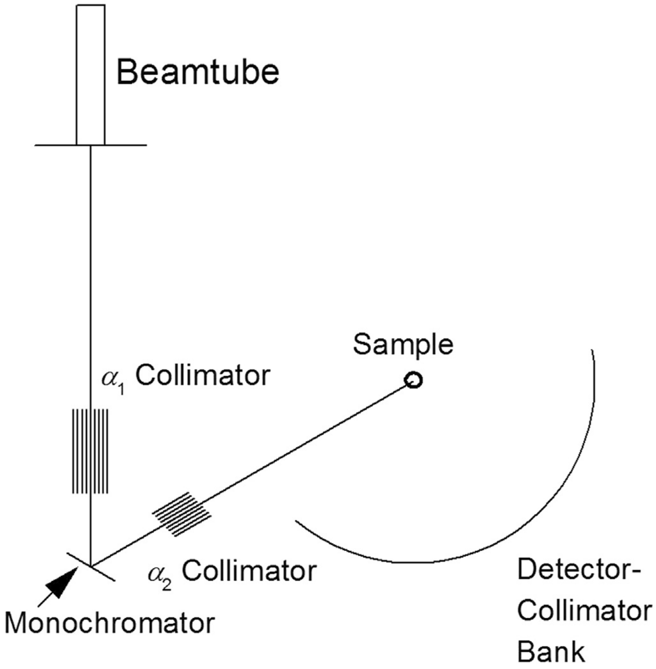

Fig. 1. Schematic illustration of the in-scattering plane instrument layout for a conventional collimated constant wavelength neutron powder diffractometer. The detector bank may include a large number of collimators and detectors or be a PSD.

It is common to consider high resolution and high intensity powder diffractometers (HRPDs and HIPDs) as distinct instrument types and to apply different design considerations to them. HIPDs often use an open geometry coupled to a PSD where the collimation is by beam tubes rather than Soller collimators. The resulting larger effective solid angle coverage after the sample greatly increases count rates. Such instruments typically have higher background (somewhat mitigated by the use of a radial oscillating collimator after the sample) and are very sensitive to the accurate centering of the sample. Using a PSD introduces some cross-talk between spatial and angular positions but this is also present in a scan on a collimated CW PD. Some believe that such open geometry instruments are incapable of measurements at the highest desirable resolutions.

3. Typical count rates on CW PD's

Neutron sources are very weak.

One illustration of this is to regard a nuclear reactor source as a bottle of "neutron gas". Comparing the measured neutron flux to the expression calculated using the kinetic theory of gases, $\Phi = \frac{1}{4} N_V v_{AV}$, shows that the most intense sources produce a tiny equivalent "neutron gas pressure" of about 10^{-8} atmospheres. A second illustration is that a 20 Watt incandescent light globe produces photons at about 100 times the rate that the world's most powerful neutron sources produce neutrons. An additional challenge in neutron instrumentation is that all common neutron optics elements (with the exception of neutron guides) condition beams by discarding unwanted neutrons. Thus, there are large losses in transmission from the already weak source to the detector. Fortunately, there is effectively no natural neutron background and ^{3}He detectors can approach 100% efficiency.