Data analysis in such cases where reflections often overlap is, however, more difficult. In the analysis of intact retinal rods, Yeager (1975) gave a detailed analysis of this problem. He obtained the background from the equatorial scattering by rotating the retina by 90° from the Bragg reflecting position. To fit a smooth curve to this background data he used polynomial functions with multiple linear-regression analysis. Peak integration was then achieved by fitting Gaussians to the background subtracted data.

The authors are indebted to many who contributed to the successful design, manufacturing and maintenance of the low-angle data-acquisition system: notably D. E. Engelman, S. Rankowitz, E. Caruso, T. Clifford, V. Radeka, G. Dimmler, P. Gileeny, L. Roger, M. Kelley and H. Okuno.

Fig. 9. Intensity contour map of a dipalmitoyl lecithin sample showing the first four orders. This sample has a lamellar spacing of 60 Å and a mosaic of 0.2°.

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References


The Converging-Beam Small-Angle Neutron Diffractometer: Calculated Resolution

By A. C. Nunes, Department of Physics, University of Rhode Island, Kingston, Rhode Island 02881, USA

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The resolution function of a converging-beam system for use in a small-angle neutron diffractometer is investigated. It is shown that beam convergence in itself has only a small effect on resolution. Also a consideration is the monochromator and the correlation between wavelength and angle which it imposes upon the beam falling on the sample. Only minor modifications of existing monochromator and shield are required to produce a converging beam.

I. Introduction

Small-Angle Neutron Scattering (SANS) is finding application in an increasing number of disciplines including physics, chemistry, biology and applied science (Schmatz, Springer, Schelten & Ibel, 1974). There appear to be two reasons for
this growing popularity. First, SANS investigates structures of a size between and overlapping those studied by traditional crystallography and electron microscopy and provides information not available through other techniques. Second, advanced SANS instruments have recently become available to the general scientific community. The fact that the demand for time on such instruments (for example, D11 at the ILL in Grenoble) has outgrown that available, has spurred the construction of new machines in the US (NSF, 1978) and Europe (ILL Annual Report, 1976). Many projects however, especially those in their early exploratory stages, do not require the high neutron flux and very sophisticated instrumentation available at a national center, and could in fact benefit from the relaxed time schedule and greater flexibility of a more modest SANS instrument at a smaller reactor. An instrument of the latter type is being planned at the University of Rhode Island (URI), for installation at the Rhode Island Nuclear Science Center (RINSC) 2 MW research reactor. This paper is concerned with the resolution of the projected instrument.

Though some useful work has been performed with instruments employing a single detector with Soller slits, step scanning the scattering pattern (Nunes, 1973; Haywood & Worcester, 1973), Position-Sensitive Neutron Detectors (PSD) (Hendricks, 1976; Alberi, Fischer, Radeka, Rogers & Schoenborn, 1975) are now commercially available, and prices of computers are dropping daily so that a SANS instrument employing these technologies can be constructed on a modest budget. In fact, replacing the detector of a conventional powder spectrometer with a PSD will result in a serviceable SANS instrument.

Space limitations and considerations of budget and instrument geometry often limit a neutron flight path to less than 3 m, and a (single slit) beam width to a few millimeters or less at the sample. The latter places severe limitations on the beam current available to an experiment. Beam focusing techniques have been demonstrated (Nunes, 1974; Nunes & Zaccai, 1975) which permit the use of broad samples and consequently higher neutron currents, apparently without compromising instrument resolution. Converging-beam techniques which require little or no modification to existing monochromator shielding and inpile collimation are particularly interesting from the point of view of cost. To investigate possible design options, a computer program was written to calculate instrument resolution.

The present paper addresses the resolution function of a SANS instrument employing a linear one-dimensional PSD set perpendicular to the incident beam, and converging-beam optics. Since detector resolution is well known (Alberi et al., 1975), only the effects of the beam optics are considered. The size of the scattered beam spot at the detector is calculated for two monochromator configurations (monochromator scattering plane perpendicular or parallel to sample scattering plane) and is compared with widths calculated for a single-slit non-converging beam geometry.

II. Resolution and focusing concepts

In this note, we are concerned with the effect of beam focusing on instrument resolution rather than the complete description of the resolution function itself. We consider the case of a neutron beam scattering from a sample, and the scattered beam illuminating a spot of width $\delta X$ on the detector at a distance $L$ from the position of the direct beam. To simplify the discussion, the detector is assumed to be linear and oriented perpendicular to the incident beam at a distance $L$ from the sample. Only resolution in one dimension is considered. The scattering angle will be

$$2\theta = \tan^{-1}(X/L)$$

and the beam angular resolution will be (ignoring effects of vertical divergence)

$$\delta(2\theta) \approx [\delta X \cos^2(2\theta)/L].$$

The key resolution parameter to be calculated is $\delta X$.

In the simplest case, the neutron source may be considered as an extended diffuse radiator. If for the moment the monochromator is ignored, the spot size and shape at the detector can be found by interposing two slits of widths $d_1$ and $d_2$ separated by a distance $L_0$, the detector being at distance $L$ from the second slit. The intensity distribution at $L$ will in general be trapezoidal with a base width $W_0$ and top width $W_1$ given by

$$W_0 = d_2 + (d_1 + d_2)L/L_0$$

$$W_1 = d_1 - d_2 L_0/L_{col}.$$  

The full width at half maximum of this trapezoid will be defined as

$$\delta X = W_0 + W_1/2.$$  

At this point it is useful to pick approximate values of $L$, $L_0$, and $\delta X$ to get an idea of the dimensions of the double slit. In the present case, the collimator length $L_0$ will be approximately 50 cm, the collimator-to-detector distance $L$ approximately 150 cm, and $\delta X$ should be of the order of the detector resolution of $\delta X \approx 5$ mm. These numbers translate into $\delta \theta \approx 0.2^\circ$ or a maximum resolvable spacing of 600 A with a neutron wavelength of 4 A. With these dimensions as design constraints, $d_1$ and $d_2$ can be no larger than 2 mm.

To increase the effective beam width at the sample without worsening angular resolution, it is possible to use a Soller array of collimating channels which converge to a point to replace the single-channel collimator. This does not increase beam flux at the sample, but does increase beam area and current at the sample, and increases neutron intensity at the detector by the number of channels in the collimator.

The intensity observed right at the point of convergence of the collimator will be the maximum possible from the available source. This is illustrated in Fig. 1. The neutron
source (the inner end of the beam tube) can be viewed as a diffuse patch of total emission proportional to its area \( A \). At a distance \( R \) from the patch, the observed neutron intensity will be \( A/R^2 \). If shielding is placed around this source with only the converging collimator piercing it, observed intensity will be zero everywhere except in the neighborhood of the axis of the collimator. At the point of convergence, all the vanes of the collimator are viewed edge on, and if they are infinitely thin, the entire source patch is seen, undiminished. It should be noted that neutron guides, focusing monochromators or mirrors placed between source and collimator can be considered as having the effect of increasing the effective source area without altering its brightness or position. With such devices one can increase the number of channels and beam area at the sample with a corresponding increase in spot intensity at the detector. Unless the original source is smaller than the area viewed through the original collimator, or is of non-uniform brightness, however, guides and focusing monochromators can yield no increase in beam flux at the sample.

The resolution function of a single-channel spectrometer as a function of scattering angle is well known, and depends in part upon the method of monochromating the neutron beam. The resolution of the multichannel converging-beam spectrometer is complicated by the fact that the distance between collimator exit (or sample position) and the beam convergence point is also a function of scattering angle, and the shape of the locus of these points is also strongly influenced by the monochromator configuration. In the next section is sketched the form of these two effects of monochromator configuration on spectrometer resolution.

III. Single and multichannel resolution

The form of the resolution function of a neutron spectrometer depends upon the correlation between wavelength and angle introduced by the monochromator system. These quantities may be very strongly correlated or completely independent and this affects both the single and multichannel parts of the resolution function of a SANS employing a converging beam.

The single-channel diffractometer resolution function has been worked out for two cases. If the wavelength and angular dispersion of the beam falling on the sample are uncorrelated, then the resolution is given by (Nunes, 1973)

\[
\delta \theta = \left[ \delta \lambda^2 + \left( \frac{\delta \lambda}{\lambda} \right)^2 \right]^{1/2},
\]

where \( \delta \lambda \) is the width of the direct beam, \( \delta \lambda \) is the width of the spectrum passed by the monochromator, \( \lambda \) is the mean wavelength, and \( \delta \theta \) is the scattering angle of the sample. This shall be called case (a). This case is approached to first order in the real world when \( \delta \lambda \) and \( \delta \theta \) are small. (a) the scattering half angle and \( A, B \) and \( C \) are constants which are positive if the sense of \( \theta \) for the sample is opposite that for the monochromator. We will consider the two cases where the resolution of one channel of a converging-beam system is described by \( (a) \) or \( (b) \), as these are the two configurations most easily duplicated with conventional apparatus.

In discussing the multichannel converging collimator, a similar convention is adopted. Case \( (a) \) denotes that for which the mean wavelength of all channels is identical. Case \( (b) \) denotes that for which the mean wavelength of the channels changes monotonically across the collimator. The former can be achieved by those arrangements described in \( (a) \) above, and a fifth additional configuration: if the monochromator and sample scattering planes are parallel and the monochromator is curved in the plane and symmetrically imaging the source on the detector (i.e. source-to-monochromator and monochromator-to-detector distances are equal). In case \( (a) \) the distance from sample (placed at the exit of the collimator) to beam-convergence point \( L_a \) is given by (Nunes & Zaccai, 1975)

\[
L_a = L_c \cos 2\theta.
\]

This is the circle (or sphere, if scattering is observed in two dimensions) familiar to users of Guinier X-ray cameras (Witz, 1969). If the beam incident on the case \( (b) \) curved monochromator is parallel, the distance between sample and beam-convergence point will be

\[
L_b = \frac{L_c \cos 2\theta}{1 - \tan(\theta) \tan(\theta_m)},
\]

where \( \theta \) and \( \theta_m \) are sample and monochromator scattering half angles respectively. Fig. 2 is a sketch of these two cases. The dotted circle is that of case \( (a) \), while the solid curve is case \( (b) \) (equation 8) caused by the straight inplane collimator and curved monochromator shown.

In the next section are presented calculations of the resolution of a projected SANS instrument for the two cases described above.

IV. Calculated beam profiles

To get an idea of the magnitude of the above effects on instrument resolution a computer program based on the pre-

![Fig. 2. Locus of beam point of convergence for two monochromator configurations: (a) dotted curve: for monochromator plane of scattering perpendicular to that of sample (not shown); (b) solid curve: for monochromator and inplane collimator as shown. (See text.)](image-url)
The main thrust of the study has been to provide information upon which to base the design of a converging neutron beam system to be used in a small-angle neutron diffractometer being built by the University of Rhode Island at the Rhode Island Nuclear Science Center. The immediate conclusion is that instrument resolution will not be significantly worsened by using a converging beam (though the gains in available beam area and current are very substantial), and that the exact configuration of the bent monochromator is not important for $2\theta \leq 15^\circ$. For a larger range of scattering angles, resolution may be made to be symmetrical about $2\theta = 0$ by mounting the linear position-sensitive detector vertically so that monochromator and sample planes of scattering will be mutually perpendicular. The only modifications required of a conventional powder diffractometer to convert it to a useful SANS instrument are: opening inpile collimation, installing a bent graphite monochromator, mounting a converging collimator, and replacing the counter with a linear position-sensitive detector.

In the broader view, it appears that any resolution penalties incurred using a converging beam system with a properly designed SANS instrument will be small, and (where space permits) to be minimally reduced by choosing as many channels as possible instead of one.

V. Conclusions

The main thrust of the study has been to provide information upon which to base the design of a converging neutron beam system to be used in a small-angle neutron diffractometer being built by the University of Rhode Island at the Rhode Island Nuclear Science Center. The immediate conclusion is that instrument resolution will not be significantly worsened by using a converging beam (though the gains in available beam area and current are very substantial), and that the exact configuration of the bent monochromator is not important for $2\theta \leq 15^\circ$. For a larger range of scattering angles, resolution may be made to be symmetrical about $2\theta = 0$ by mounting the linear position-sensitive detector vertically so that monochromator and sample planes of scattering will be mutually perpendicular. The only modifications required of a conventional powder diffractometer to convert it to a useful SANS instrument are: opening inpile collimation, installing a bent graphite monochromator, mounting a converging collimator, and replacing the counter with a linear position-sensitive detector.

In the broader view, it appears that any resolution penalties incurred using a converging beam system with a properly designed SANS instrument will be small, and (where space permits) to be minimally reduced by choosing as many channels as possible instead of one.
and budgetary restrictions are severe) are far outweighed by gains in available beam area and current. This supports the qualitative observations of previous work (Nunes, 1974). It is hoped that this study will help to stimulate the proliferation of SANS instruments as, in this author's opinion, the full potential of this very valuable technique is yet to be realized.

References


Design Study of a Time-of-Flight Small-Angle Diffractometer for a Pulsed Neutron Source*

(Extended Abstract only) By J. M. Carpenter and J. Faber Jr, Argonne National Laboratory, Argonne, Illinois 60439, USA

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A design study was made of a neutron small-angle scattering (SAS) instrument for use at Argonne National Laboratory's proposed Intense Pulsed Neutron Source, IPNS-II (Carpenter & Werner, 1976; Werner, 1977; Carpenter, 1977). The instrument design incorporates several features: a converging-slit collimator, wavelength band-limiting choppers, capacity for large samples, and a two-dimensional detector. Machine design-dependent parameters are considered in a Monte-Carlo code that produces estimates of the instrumental resolution function and available flux at the sample. It was found that the calculated flux on sample exceeds that at steady-state reactor instruments of comparable resolution.

Pulsed neutron sources can provide higher effective neutron fluxes than are available at high-flux research reactors (e.g. the peak thermal flux at IPNS-II is $10^{16} \text{ n cm}^{-2} \text{ s}^{-1}$). Most measurements currently performed use very efficient instruments based on steady-state monochromatic neutron beams; however, the increasing need for neutron SAS instrumentation and the advent of next-generation pulsed sources dictate the further development of neutron SAS facilities that utilize time-of-flight (TOF) techniques. Recently, at Dubna (Cser, 1975) and Harwell (Mildner & Windor, 1978), TOF instruments have been tested at pulsed neutron sources.

A schematic design of the neutron (TOF) instrument is shown in Fig. 1, and appears to resemble a steady-source instrument. However, in the steady-state instrument, the incident wavelength $\lambda_0$ is fixed by a crystal or drum velocity selector and a range of wave-vector change $Q = 2\pi/\lambda_0 (\Omega_i - \Omega_j)$ is scanned by an array of detectors. Here $\Omega_i$ and $\Omega_j$ are incident and scattered neutron direction vectors. In the time-of-flight instrument, a wide range of incident wavelengths is used, and the time at which neutrons started at the pulsing device is known. Neutrons are sorted by wavelength according to their time of flight $t = (m/h)\lambda$ across the known path $L = [L_1 = L_2(\Omega)]$ and the wave-vector change $Q$ for each wavelength $\lambda$ is determined for each direction $\Omega_j$. Since a wide band of wavelengths is used, the time-of-flight instrument spans a greater range of $Q$ than a steady-state instrument with the same angular range.

The two-dimensional converging-slit collimator (represented in the figure only by the entrance and exit apertures) consists of channels which converge at a point on the detector and is incorporated to increase the area of source and sample that can be used in a small-angle scattering instrument. There is negligible sacrifice in resolution. Thus, for a source having 10 x 10 cm area, the sample area may be as large as 5 x 5 cm. The wavelength range is great enough to enable a large range of $Q$ to be covered in a single run, but is restricted by the condition against 'frame overlap' (faster neutrons from one pulse may not overtake slower ones from a previous pulse). The condition is

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