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An Optimized Monte Carlo Simulation for Diffraction Experiments Using Pulsed Neutron Sources*

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The method of determining corrections to neutron time-of-flight diffraction data by Monte Carlo techniques is costly since a large range of neutron wavelengths must be considered. An optimized simulation is presented in which many wavelengths are considered simultaneously, while paths are traced only once for all wavelengths. Collision positions and scattering angles are selected from cumulative distribution functions representing all neutron wavelengths simulated. The scattered intensity is computed by weighting the simulated paths to account for the probability of their occurrence for each wavelength. The results of a calculation for a vanadium slab are given as an example.

1. Introduction

In the previous paper (Mildner, Pelizzari & Carpenter, 1977) a simple but optimized Monte Carlo simulation of a neutron diffraction experiment was presented so that multiple scattering corrections could be estimated. This program is most suitable for the 'reactor' experiment in which a beam of neutrons with a unique wavelength obtained from a crystal monochromator is scattered by the specimen, and the diffracted intensity is measured as a function of scattering angle. Following the Bischoff (1970) algorithm, it is natural to think of calculating the scattering and escape probabilities for each of many scattering angles at each collision point on the path of a neutron of given wavelength. However to apply a multiple-scattering correction to time-of-flight diffraction data, it is necessary to perform the simulation for the large range of wavelengths available to the diffractometer, but at only one or perhaps a small number of scattering angles. Since correction factors are required as a function of scattering vector Q, this operation becomes formidable and judicious choices of neutron wavelengths are required to reduce computing time. The simulation is performed for a certain number of values of Q (and hence wavelengths), with a higher density of points in regions of Q where the structure factor $S(Q)$ varies greatly. (An example of the computation of multiple scattering corrections for time-of-flight diffraction of an isotropic system is given in the previous paper, and shows that the correction factor is not featureless). However, we describe here a method by which this operation may be made more efficient.

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In the case of the unique wavelength simulation of the conventional diffraction experiment, the positions of the scattering events and the directions of scatter are determined from the cumulative distribution functions of path lengths and scattering angles for that particular wavelength. However in this work we present a simulation in which a 'neutron' does not have a unique wavelength, but rather there are many wavelengths as in a diffraction experiment using a pulsed neutron source. Once generated, the paths are assumed to be travelled by neutrons having as many wavelengths as desired. One way to approach an optimized simulation is to select collision positions and scattering angles from cumulative distribution functions for some weighted distribution of neutron wavelengths, and to calculate the detector scores with this distribution taken into account. The basic ideas of the Monte Carlo computations of Bischoff (1970) have been extended, for instead of thinking of the simulation as one which follows 'neutrons', it is more efficient to consider the simulation as one which generates paths in the scatterer, while probabilities of various events are computed for many neutron wavelengths for each path.

The time-of-flight diffraction experiment uses a continuous distribution of neutron wavelengths which are scattered into various detectors at particular scattering angles, and the experiment is analyzed by time-of-flight techniques in order to obtain a scattered intensity as a function of scattering vector. For a neutron of a particular wavelength λ_i scattered elastically through an angle θ_j, the corresponding scattering vector Q_{ij} is given by

$$Q_{ij}=4\pi/\lambda_i \sin \theta_j/2 . \qquad (1)$$

Rather than consider a continuous distribution of wavelengths, the simulation considers particular wavelengths each with its own relative weighting factor.

Comments on the choice of these factors are left until later.

The reader is referred to the earlier paper for details common to the unique-wavelength and the present multi-wavelength calculations.

2. Scattering path length distribution

Throughout the simulation collision points within the sample must be chosen which reflect the relative importance of each wavelength λ_i with its own total cross section $\Sigma_T(\lambda_i)$. We refer to Fig. 1 of the previous paper. The distance l_n from the previous scattering point to the nth collision point is chosen from the distribution

$$F(l_n)=\frac{\sum_i w_i \int_0^{l_n} \exp\left[-\Sigma_T(\lambda_i)l\right]\mathrm{d}l}{\sum_i w_i \int_0^{t_n} \exp\left[-\Sigma_T(\lambda_i)l\right]\mathrm{d}l}, \tag{2}$$

where t_n is the maximum distance that the neutron can travel within the sample in the direction $\mathbf{\Omega}_n$ which was obtained at the previous, $(n-1)$th, scattering point. The summation extends over all wavelengths λ_i, each with its relative weighting factor w_i. Performing the integrals, we obtain the path length distribution function

$$F(l_n)=\frac{\sum_i w_i/\Sigma_T(\lambda_i)\{1-\exp\left[-\Sigma_T(\lambda_i)l_n\right]\}}{\sum_i w_i/\Sigma_T(\lambda_i)\{1-\exp\left[-\Sigma_T(\lambda_i)t_n\right]\}}. \tag{3}$$

So that the selection of the collision point is done optimally, prior to the running of the neutron histories an array $G(l)$ must be set up with the elements

$$G(l)=\sum_i w_i/\Sigma_T(\lambda_i)\{1-\exp\left[-\Sigma_T(\lambda_i)l\right]\} \tag{4}$$

for incremental values of l in steps of Δl, with the maximum value of l at least as large as the greatest possible length within the sample under discussion. Then the cumulative path length distribution function is given by

$$F(l_n)=G(l_n)/G(t_n). \tag{5}$$

When a random number R_{ln} has been selected, the determination of the collision point is performed by searching through $G(l)$ until a value l_m is found for which

$$F(l_m)\le R_{ln}<F(l_{m+1}), \tag{6}$$

as shown schematically in Fig. 2 of the previous paper. That is

$$G(l_m)\le R_{ln}G(t_n)<G(l_{m+1}). \tag{7}$$

Then the distance between successive collision points is given by

$$l_m\le l_n<l_{m+1} \tag{8}$$

and, by linear interpolation,

$$l_n=l_m+\Delta l\frac{R_{ln}G(t_n)-G(l_m)}{G(l_{m+1})-G(l_m)}. \tag{9}$$

Since all the scattering events are forced to occur within the sample, and since the path length distribution function given by (3) is not exact for any particular wavelength, then the worth of each 'neutron' must be modified after each collision point has been selected. The modification factor accounts for the procedure of selecting the scattering path lengths from the distribution, and is equal to the ratio of the true probability of reaching the selected scattering point to the probability that the scattering path length is drawn from the distribution. However the factors are not simple since the distribution from which the collision points are selected is not uniform; on the other hand, the random numbers from which the path lengths are chosen are selected from a uniform distribution. The random number R_{ln} in the interval (0,1) is made equal to the cumulative distribution $F(l_n)$ for the path length l_n, so that

$$R_{ln}=F(l_n)=G(l_n)/G(t_n). \tag{10}$$

Then the probability that the scattering path length l_n is selected is given by

$$\frac{\mathrm{d}R_{ln}}{\mathrm{d}l_n}=\frac{\mathrm{d}F(l_n)}{\mathrm{d}l_n}=\frac{1}{G(t_n)}\frac{G(l_n)}{\partial l_n}. \tag{11}$$

The true probability of a neutron of wavelength λ_k scattering at a distance l_n is given by $\Sigma_s(\lambda_k)\exp\left[-\Sigma_T(\lambda_k)l_n\right]$, so that the factor H_{nk} by which the 'neutron' worth of each wavelength λ_k is modified to account for the method of selection of the nth scattering path is given by

$$H_{nk}=\frac{\Sigma_s(\lambda_k)\exp\left[-\Sigma_T(\lambda_k)l_n\right]}{\frac{1}{G(t_n)}\frac{\partial G(l_n)}{\partial l_n}}. \tag{12}$$

Fortunately the array $G(l)$ is defined explicitly in terms of l by (4), so that the factor H_{nk} may be expressed as

$$H_{nk}=\frac{\Sigma_s(\lambda_k)\exp\left[-\Sigma_T(\lambda_k)l_n\right]\sum_i w_i/\Sigma_T(\lambda_i)\{1-\exp\left[-\Sigma_T(\lambda_i)t_n\right]\}}{\sum_i w_i\exp\left[-\Sigma_T(\lambda_i)l_n\right]}. \tag{13}$$

Then for the unique λ case, this factor reduces to

$$\frac{\Sigma_s(\lambda_k)}{\Sigma_T(\lambda_k)}\{1-\exp\left[-\Sigma_T(\lambda_k)t_n\right]\}$$

which is identical to that found in the unique wavelength simulation, where $\{1-\exp[-\Sigma_T(\lambda_k)t_n]\}$ is the non-escape probability for the neutron of wavelength λ_k within the distance t_n and the factor $\Sigma_s(\lambda_k)/\Sigma_T(\lambda_k)$ is the probability that the collision is a scattering process.

3. Scattering angle distribution

At each collision point in the simulation a scattering angle must be chosen which reflects the relative importance of each wavelength λ_i with its own differential cross section $\partial\sigma/\partial\Omega(\lambda_i)$. The scattering angle θ_n at the nth scattering event is chosen from the distribution

$$f(\theta_n)=\frac{\sum_i v_i \int_0^{\theta_n} \frac{\partial\sigma}{\partial\Omega}(\theta',\lambda_i)\sin\theta' d\theta'}{\sum_i v_i \int_0^{\pi} \frac{\partial\sigma}{\partial\Omega}(\theta',\lambda_i)\sin\theta' d\theta'}. \quad (14)$$

Note that there is no reason that the relative weighting factors v_i used in computing $f(\theta_n)$ must be the same as the w_i used for computing $F(l_n)$. Though it may be natural, lacking any compelling reason otherwise, to make them equal, we maintain generality by keeping them unequal.

For any particular scattering angle θ_j, the corresponding scattering vector Q_{ij} is a function of wavelength λ_i given by (1); hence the selection of the scattering angle cannot be obtained by a simple summation of the first moment of the diffraction pattern as in the unique-wavelength case. Again prior to the running of the neutron histories, an array $g(\theta)$ must be set up with elements

$$g(\theta_m)=2\pi\sum_i v_i \sum_{j=1}^{m} \frac{\partial\sigma}{\partial\Omega}(\theta_j,\lambda_i)\sin\theta_j\Delta\theta_j \quad (15)$$

where $\Delta\theta_j$ is the incremental step in the value of θ_m. Then the cumulative scattering angle distribution function is given by

$$f(\theta_n)=g(\theta_n)/g(\pi), \quad (16)$$

where the maximum value of the array is

$$g(\pi)=2\pi\sum_i v_i \sum_{j=1}^{\theta_j=\pi} \frac{\partial\sigma}{\partial\Omega}(\theta_j,\lambda_i)\sin\theta_j\Delta\theta_j=\sum_i v_i\sigma_s(\lambda_i). \quad (17)$$

Since diffraction data are usually expressed as functions of scattering vector Q rather than scattering angle θ (conventional diffraction) or wavelength λ (time-of-flight diffraction), we recast the above functions in terms of the scattering vector rather than the scattering angle. From (1), we obtain

$$Q_{ij}\Delta Q_{ij}=4\pi^2/\lambda_i^2\sin\theta_j\Delta\theta_j. \quad (18)$$

The differential cross section $\partial\sigma(\theta,\lambda)/\partial\Omega$ and the structure factor $S(Q)$ are related by

$$\frac{\partial\sigma}{\partial\Omega}(\theta_j,\lambda_i)=S(Q_{ij}), \quad (19)$$

where we have included the square of the scattering length in our $S(Q)$. (15) may be written

$$g(\theta_m)=(1/2\pi)\sum_{j=1}^{m}\sum_i (v_i\lambda_i^2)S(Q_{ij})Q_{ij}\Delta Q_{ij}. \quad (20)$$

Though it is advantageous to use $S(Q)$ as a function of Q rather than to use $\partial\sigma(\theta_j,\lambda_i)/\partial\Omega$ as input to the calculation, a given scattering angle of course gives a different Q for each wavelength. Consequently the array element $g(\theta_m)$ is expressed in terms of $S(Q_k)$ (assumed to be tabulated on intervals ΔQ_k) and within the summation of wavelengths λ_i the sum on Q_k runs to the limit $Q_m^*(\lambda_i)$ which is a function of λ_i; that is,

$$g(\theta_m)=(1/2\pi)\sum_i (v_i\lambda_i^2)\sum_k S(Q_k)Q_k\Delta Q_k, \quad (21)$$

$$k \text{ such that } 0\le Q_k\le Q_m^*(\lambda_i),$$

where

$$Q_m^*(\lambda_i)=4\pi/\lambda_i\sin\theta_m/2. \quad (22)$$

This function $g(\theta_m)$ needs to be computed only once before the summation and any mesh of Q and ΔQ can be dealt with.

At the nth scattering event we select a random number $R_{\theta n}$, and the determination of the scattering angle is performed by searching through $g(\theta_m)$ until a value θ_m is found for which

$$f(\theta_m)\le R\theta_n<f(\theta_{m+1}), \quad (23)$$

as shown schematically in Fig. 1. That is,

$$g(\theta_m)\le R_{\theta n}g(\pi)<g(\theta_{m+1}). \quad (24)$$

Then the scattering angle is given by

$$\theta_m\le\theta_n<\theta_{m+1} \quad (25)$$

and, by linear interpolation,

$$\theta_n=\theta_m+\Delta\theta\frac{R_{\theta n}g(\pi)-g(\theta_m)}{g(\theta_{m+1})-g(\theta_m)}. \quad (26)$$

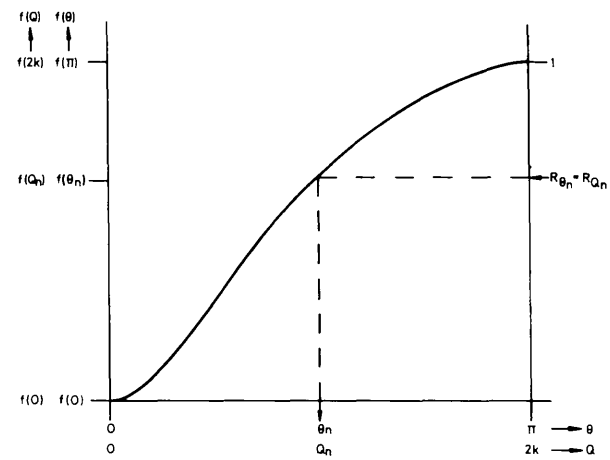

Fig. 1. The selection of the nth scattering angle from the cumulative distribution of scattering angles, $f(\theta)$, and hence the corresponding wave vector transfer.

Since the scattering angle distribution function given by (14) is not exact for any particular wavelength, then again the worth of each 'neutron' must be modified after each scattering angle has been selected. The modification factor accounts for the procedure of selecting the scattering angle from the distribution, and is equal to the ratio of the true probability of scattering at the particular angle to the probability that the scattering angle is drawn from the distribution. Again, the factors are not simple since the distribution from which the scattering angles are selected is not uniform; on the other hand, the random numbers from which the scattering angles are chosen are selected from a uniform distribution.

The random number $R_{\theta n}$ in the interval (0, 1) is made equal to the cumulative distribution $f(\theta_n)$ for the scattering angle θ_n, so that

$$R_{\theta n} = f(\theta_n) = g(\theta_n)/g(\pi) . \tag{27}$$

Then the probability that the scattering angle θ_n is selected is given by

$$\frac{\mathrm{d}R_{\theta n}}{\mathrm{d}\theta_n} = \frac{\mathrm{d}f(\theta_n)}{\mathrm{d}\theta_n} = \frac{1}{g(\pi)} \frac{\partial g(\theta_n)}{\partial \theta_n} . \tag{28}$$

The true probability of a neutron of wavelength λ_k scattering by an angle θ_n is given by

$$\frac{2\pi}{\sigma_s(\lambda_k)} \frac{\partial \sigma}{\partial \Omega}(\theta_n, \lambda_k) \sin \theta_n ,$$

so that the factor h_{nk} by which the 'neutron' worth of each wavelength λ_k is modified to account for the method of selection of the nth scattering angle is given by

$$h_{nk} = \frac{\dfrac{2\pi}{\sigma_s(\lambda_k)} \dfrac{\partial \sigma}{\partial \Omega}(\theta_n, \lambda_k) \sin \theta_n}{\dfrac{1}{g(\pi)} \dfrac{\partial g(\theta_n)}{\partial \theta_n}} . \tag{29}$$

The factor represents the modification to the weight to account for the fact that the scattering directions are chosen from the distribution $f(\theta)$ rather than from the one correct for the wavelength λ_k. If the chosen direction happens to be a particularly likely (or unlikely) one for λ_k, then the neutrons on that path are weighted heavily (or lightly) compared to the weight built into the simulation through the distribution $f(\theta)$. In fact the factor h_{nk} may be greater than unity. Fortunately the array $g(\theta_n)$ is defined explicitly in terms of θ_n by (15), so that the factor h_{nk} may be expressed as

$$h_{nk} = \frac{\sum_i v_i \sigma_s(\lambda_i)}{\sigma_s(\lambda_k)} \frac{\partial \sigma(\theta_n, \lambda_k)/\partial \Omega}{\sum_i v_i \partial \sigma(\theta_n, \lambda_i)/\partial \Omega} , \tag{30}$$

or in terms of the corresponding scattering vector

$$h_{nk} = \frac{\sum_i v_i \sigma_s(\lambda_i)}{\sigma_s(\lambda_k)} \frac{S(Q_{n,k})}{\sum_i v_i S(Q_{n,i})} . \tag{31}$$

For the unique-wavelength case, this factor reduces to unity, of course, since the scattering angles are selected from the correct distribution.

It should be observed that throughout this simulation, it has been assumed that the scattering is independent of azimuthal angle φ, and hence the distribution of azimuthal angles is not only uniform but also independent of wavelength. Consequently the probability of scattering with a particular azimuthal angle is equal to the probability that that azimuthal angle is drawn from the distribution of azimuthal angles. Hence the random number $R_{\varphi n}$, in the interval (0, 1) uniquely determines the azimuthal angle φ_n of the scattered direction after the nth scattering point by

$$\varphi_n = 2\pi R_{\varphi n} . \tag{32}$$

After each collision the weight of the history for each wavelength is adjusted:

$$W_{nk} = W_{(n-1)k} H_{nk} h_{nk} . \tag{33}$$

When $W_{0k} = 1/\sigma_s(\lambda_k)$ the computed scores represent the probabilities for scattering of neutrons of various wavelength into the detectors.

4. Scoring

Now the Monte Carlo simulation of paths needs be performed only once instead of N times, where N is the number of wavelengths that are being considered. Admittedly neither the scattering points nor the scattering angles are chosen optimally for any wavelength; but this has been compensated by modification factors or statistical weights in the 'neutron' worth. Nevertheless this method provides a large saving in the computing time, since only one Monte Carlo simulation of an ensemble of paths is required. It is to be expected that a somewhat larger number of paths needs to be simulated in the multi-wavelength calculation than in the unique-wavelength case to obtain the required statistical accuracy; however this increase is not nearly a factor of N.

To adapt the simulation of the monochromatic case to that for the pulsed source, arrays $G(l)$ and $g(\theta)$ must be set up. In addition various parameters must be given an extra dimension of N. Principally, this involves the scattering and total cross sections, the statistical weights of the neutrons of various wavelengths and also the scores of the various detectors.

The score $S_{n,k}(\theta_D)$ of the neutron of wavelength λ_k scattering with n collisions into a detector at a scattering angle θ_D subtending an angle $\Delta\boldsymbol{\Omega}_D$ at the sample is not dependent on the cumulative scattering distribution at the nth scatter, but rather on the particular differential scattering probability $p_{Dn}(\lambda_k)$ given by

$$p_{Dn}(\lambda_k) = \frac{\Delta\Omega_D}{\sigma_s(\lambda_k)} \frac{\partial \sigma}{\partial \Omega}(\theta_{Dn}, \lambda_k) , \tag{34}$$

where θ_{Dn} is the angle between the direction $\boldsymbol{\Omega}_n$ before the nth scatter and the detector direction $\boldsymbol{\Omega}_D$; that is,

$\cos\theta_{Dn} = \mathbf{\Omega}_D \cdot \mathbf{\Omega}_n$. This differential scattering probability may be simply expressed by

$$p_{Dn}(\lambda_k) = \frac{\Delta\Omega_D}{\sigma_s(\lambda_k)} S(Q_k^{Dn}), \quad (35)$$

where the scattering vector from direction $\mathbf{\Omega}_n$ into $\mathbf{\Omega}_D$ for the wavelength λ_k is given by

$$Q_k^{Dn} = 4\pi/\lambda_k \sin(\theta_{Dn}/2). \quad (36)$$

The score is also dependent on the statistical weight W_{nk} after the nth scattering position has been chosen, and on the escape probability through a distance $L_{Dn}(\mathbf{r}_n, \mathbf{\Omega}_D)$ from the point of scatter $\mathbf{r}_n$ to the edge of the target in the detector direction $\mathbf{\Omega}_D$. Hence the score is given by

$$\mathscr{S}_{n,k}(\theta) = W_{nk} p_{Dn}(\lambda_k) \exp[-\Sigma_T(\lambda_k) L_{Dn}]. \quad (37)$$

Throughout the simulation, the worth W_{nk} of a 'neutron' for each wavelength λ_k becomes smaller at each collision. Since the simulation has not been optimized for any one neutron wavelength, it is necessary to compute a weighted average of the neutron worth to determine the end of the history of the neutron. This weighted average is given by

$$W_n = \sum_i u_i W_{ni} / \sum_i u_i, \quad (38)$$

where u_i is the relative weight of a particular wavelength λ_i. When the value of W_n falls below some cut-off value $W_{\min}$, then there is half chance of the neutron history being terminated, and a half chance that the worth is increased by a factor of two. This method of Russian roulette discontinues a neutron's history without biasing the result of the simulation.

There remains the problem of selecting the *a priori* weighting factors w_i, v_i, u_i, since they give the relative importance of each wavelength in the simulation. Perhaps w_i should be proportional to the absorption cross section which is directly proportional to the neutron wavelength. Presently these weighting factors are left in their most general form, and it may be that, lacking any special reason for choosing them in some other way, the weighting factors should be chosen equally.

5. Example calculation for a vanadium slab

The scattering from a slab of vanadium [frequently used as a reference scatterer in time-of-flight (TOF) diffraction measurements] was computed using the TOF optimized code for 25 wavelengths. The arrangement calculated is shown in Fig. 2. The slab is large in extent and the beam spot small, in order to represent an 'infinite' slab. Cross sections assumed were $\sigma_s = 5{\cdot}13$ b atom^{-1} (constant and totally incoherent), σ_a (2200 m s^{-1}) = 5·06 b atom^{-1}, and the number density of scatterers 0·0722 atom b^{-1} cm^{-1}. The 'ideal', single, multiple and total scattering probabilities per unit solid angle ($\Delta\Omega_D = 1$ sterad) for scattering angle $\theta_s = 30°$ are shown in Fig. 3. Correction factors for attenuation, multiple scattering and the net of both effects are shown in Fig. 4. Data processed as though the scattering were 'ideal' (no attenuation or multiple scattering) are to be corrected by dividing by these factors.

The same calculation was performed with the unique wavelength code, so as to determine the computing time savings. For one wavelength, computing time on

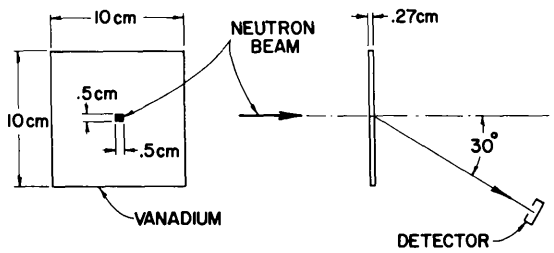

Fig. 2. The arrangement of vanadium sample, detector and neutron beam for which the scattering was calculated. It was assumed that $\sigma_s = 5{\cdot}13$ b atom^{-1} (constant and totally incoherent), σ_a (2200 m s^{-1}) = 5·06 b atom^{-1}, and that the number density of scatterers was 0·0722 atom b^{-1} cm^{-1}.

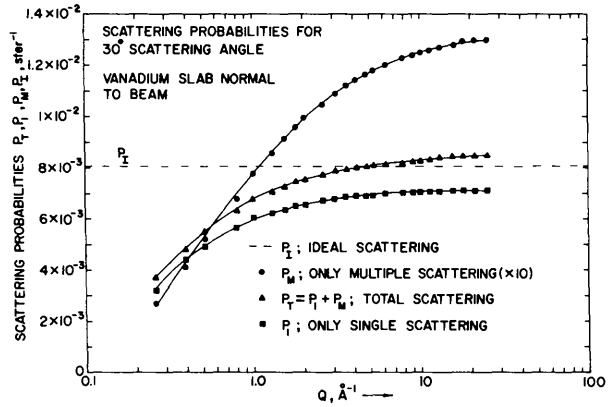

Fig. 3. 'Ideal', single, multiple and total scattering probabilities per unit solid angle computed for a scattering angle of 30°, for the arrangement of Fig. 2.

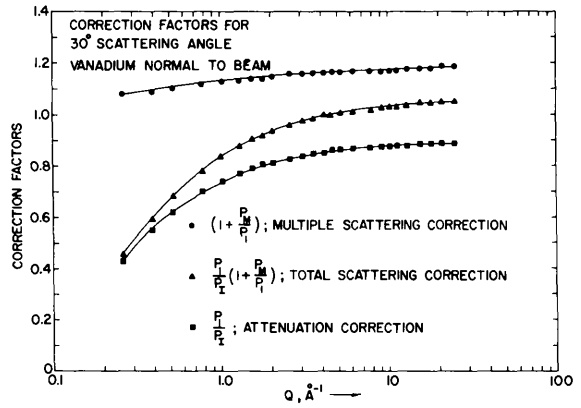

Fig. 4. Correction factors for attenuation, multiple scattering and the net of both effects computed for a scattering angle of 30°, for the arrangement of Fig. 2.

the Argonne Laboratory IBM 370/195 system was 2·77 s; computing N wavelengths with this code would require $2{\cdot}77 \times N$ s. With the multi-wavelength code, the time was found to be $(3{\cdot}0+0{\cdot}4 \times N)$ s. Therefore the cost saving to compute for large numbers of wavelengths is a factor of $2{\cdot}77/0{\cdot}4=7$.

6. Conclusion

We have presented a method by which time-of-flight diffraction data may be simulated in order to obtain corrections for multiple scattering. In the multi-wavelength case, all we wish to do is avoid going through the Monte Carlo simulation for each wavelength individually, and instead to do it just once. The idea is to choose scattering points and directions from distributions which represent somehow all the particular wavelengths being considered, and then compute scores in detector directions in such a way as not to bias the results. Thus, each scattering point and direction is to be chosen from composite cumulative distributions of scattering points and scattering angles, and yet to compensate for their not being the exact distributions for any particular wavelength the worth of the 'neutron' must be modified for each wavelength after each selection of scattering point and scattering angle. With the present methods, there is no constraint against accurate calculation of multiple scattering and attenuation corrections for time-of-flight diffraction measurement on isotropic materials, other than those imposed by the accuracy of input data. These ideas may be used for the determination of similar algorithms for the evaluation of inelastic scattering data using a spectrometer in an inverse geometry mode on a pulsed neutron source.

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Utilisation des Paramètres de Stokes dans le Calcul de l'Etat de Polarisation d'un Faisceau de Rayons X Après Diffraction par un Cristal Mosaïque

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The polarization state of an X-ray beam diffracted by a mosaic crystal is determined. The state of the incident beam being described by four Stokes parameters, the matrix method used allows the calculation of the Stokes parameters of a monochromatic X-ray beam and it leads to a general expression of the polarization factor which can be used for any polarization state of the incident beam.

Introduction

Pour calculer l'intensité diffractée par un cristal, on suppose presque toujours le rayonnement issu du tube comme non polarisé, en particulier lorsqu'on utilise comme source de rayons X la raie caractéristique d'un élément. Ce rayonnement peut être alors considéré comme la somme de deux rayonnements polarisés perpendiculairement de même intensité, et il est facile de calculer le facteur de polarisation quand on interpose un monochromateur entre le cristal et la source de rayons X. Ce calcul a été fait de façon complète lorsque le cristal et le monochromateur sont idéalement imparfaits (Whittaker, 1953; Azaroff, 1955).

Une onde électromagnétique et en particulier un faisceau de rayons X, est dite polarisée elliptiquement si le champ électrique **E** associé à cette onde peut s'écrire sous la forme:

$$\left.\begin{aligned} E_x &= a\cos(kz-\omega t) \\ E_y &= b\cos(kz-\omega t+\delta) \end{aligned}\right\}. \qquad (1)$$

Ox, Oy, Oz définissant un repère orthonormé, l'onde se propageant selon Oz. Un rayonnement polarisé elliptiquement est caractérisé par quatre quantités appelées paramètres de Stokes fonction des amplitudes a et b et du déphasage δ

$$\hat{I}=a^2+b^2,\ \hat{P}_1=a^2-b^2,\ \hat{P}_2=2ab\cos\delta,\ \hat{P}_3=2ab\sin\delta \qquad (2)$$

liées par la relation $\hat{I}^2=\hat{P}_1^2+\hat{P}_2^2+\hat{P}_3^2$.

Lorsque $a=b$ et $\delta=\frac{1}{2}m\pi$ avec $m=\pm(2n+1)$, le