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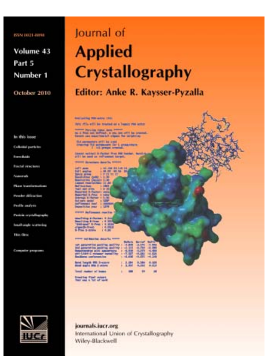

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Efficiency in the calculation of absorption corrections for cylinders

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Efficiency in the numerical calculation of absorption corrections for cylinders has been examined. Two mathematical expressions for the correction factors have been evaluated by two methods for numerical integration. It has been found that the Gauss–Legendre quadrature applied to the formula proposed by Thorkildsen & Larsen [*Acta Cryst.* (1998), A**54**, 172–185] gives results with relative errors $\leq 10^{-6}$, using 12×12 terms in the numerical integration. The conventional approach, using Simpson's method in conjunction with the formula given by Dwiggins [*Acta Cryst.* (1975), A**31**, 146–148] for the absorption correction, is far less efficient.

1. Introduction

Recently, powder diffraction measurements using capillary specimens have become more popular, in accord with expanded usage of synchrotron X-ray sources and/or high-performance X-ray detection systems, including one- or two-dimensional X-ray detectors. The effect of absorption on the diffraction intensity from a powder sample filled into a thin capillary tube can be modelled by that of cylinder, if homogeneities of the incident X-ray beam intensity and the filling factor of the powder are assumed. A numerical table listing absorption correction factors $A^*(\mu R, \theta)$ for cylinders is given as Table 6.3.3.2 in *International Tables for Crystallography*, Vol. C (Maslen, 1999), where μ is the linear absorption coefficient, R the radius of the cylinder and θ the Bragg angle. The absorption correction factor is identical to the reciprocal of the overall transmission coefficient $A(\mu R, \theta)$ of a cylinder, which has been evaluated using Simpson's numerical integration method with 101×101 terms, applied to the formula for a two-dimensional integral proposed by Dwiggins (1975). The formula of Dwiggins is given by

$$A(\mu R, \theta) = \frac{4}{\pi} \int_0^{\pi/2} \int_0^1 x \exp\Big(-\mu R \big\{ \big[1 - x^2 \sin^2(\theta + \varphi)\big]^{1/2} + \big[1 - x^2 \sin^2(\theta - \varphi)\big]^{1/2} \big\}\Big) \cosh(2\mu R x \sin\theta \sin\varphi) \, \mathrm{d}x \, \mathrm{d}\varphi. \quad (1)$$

The accuracy of the listed values, having relative errors of less than 0.1% for $\mu R \in (0, 2.5)$, is sufficient for most purposes, taking into account that the observed integrated intensities typically have relative errors of the order of 10^{-2}. However, the above formula is not favourable for numerical evaluation of the integral, because a weak singularity of the integrand exists at $x = 1$ and $\varphi = \pi/2 - \theta$, where the first derivative of the integrand approaches infinity.

Thorkildsen & Larsen (1998*a*,*b*) proposed another formula for evaluating the transmission coefficient of cylinder, given by

$$A(\mu R, \theta) = \frac{2}{\pi \sin 2\theta} \int_0^{2\theta} \int_0^{\pi - 2\theta} \exp\left[-\frac{2\mu R \sin x \cos(y - \theta)}{\cos\theta}\right] \times \sin(x + y) \sin(x - y + 2\theta) \, \mathrm{d}x \, \mathrm{d}y. \quad (2)$$

In the limits $\theta \to 0$ and $\pi/2$, the above formula is replaced by

$$A(\mu R, 0) = \frac{2}{\pi} \int_0^{\pi} \exp(-2\mu R \sin x) \sin^2 x \, \mathrm{d}x, \quad (3)$$

$$A\Big(\mu R, \frac{\pi}{2}\Big) = \frac{1}{2\pi\mu R} \int_0^{\pi} [1 - \exp(-4\mu R \sin x)] \sin x \, \mathrm{d}x. \quad (4)$$

In this communication, the results of an investigation of accuracy and convergence behaviour using an increasing number of terms in the numerical integral to evaluate the transmission coefficient of cylinders, applying the two formulae given by equations (1) and (2), and two numerical methods, Simpson and Gauss–Legendre quadratures, are reported. It will be shown that the Gauss–Legendre quadrature applied to the formula proposed by Thorkildsen & Larsen (1998*a*,*b*) given by equation (2) is much more efficient than Simpson's method applied to the conventional formula given by equation (1).

2. Numerical method

The numerical evaluation of the two-dimensional integral for the integrand function $f(x,y)$ was simply calculated by the following common formula:

$$\int_A^B \int_C^D f(x, y) \, \mathrm{d}y \, \mathrm{d}x \simeq (B - A)(D - C) \sum_{i=0}^{N-1} \sum_{j=0}^{N-1} w_i w_j f(x_i, y_j), \quad (5)$$

where $x_i = A + (B - A)\rho_i$ and $y_j = C + (D - C)\rho_j$, for abscissae $\{\rho_i\}$ normalized to the region [0, 1] and weight factors $\{w_i\}$, uniquely determined depending on the method of quadrature and the number of terms N.

Abscissae and weights for Simpson's quadrature are given by

$$\rho_i = i/(N - 1), \quad (6)$$

$$w_i = \begin{cases} 1/3N & \text{for } i = 0,\ N - 1; \\ 4/3N & \text{for } i \text{ odd}; \\ 2/3N & \text{otherwise}. \end{cases} \quad (7)$$

Table 1
Abacissae and weight factors for eight-term (N = 8) and 12-term (N = 12) Gauss–Legendre integrals.

Values for $N/2 \le j < N$ are given by $\rho_j = 1 - \rho_{N-1-j}$ and $w_j = w_{N-1-j}$.

	j	ρ_j	w_j
N = 8	0	0.019855071751232	0.050614268145188
	1	0.101666761293187	0.111190517226687
	2	0.237233795041836	0.156853322938943
	3	0.408282678752175	0.181341891689181
N = 12	0	0.009219682876640	0.023587668193254
	1	0.047941371814763	0.053469662967441
	2	0.115048662902848	0.080039164271149
	3	0.206341022856691	0.101583713361521
	4	0.316084250500910	0.116746268269177
	5	0.437383295744266	0.124573522906701

Table 2
Number of terms N needed to obtain the values of the transmission coefficients for μR = 1 within relative errors of ε.

The final column lists the exact values of the absorption correction for μR = 1.

Formula	Dwiggins (1975)					Thorkildsen & Larsen (1998*a*)					
Method	Simpson		Gauss–Legendre			Simpson		Gauss–Legendre			
ε	10^{-3}	10^{-4}	10^{-4}	10^{-5}	10^{-6}	10^{-3}	10^{-4}	10^{-4}	10^{-5}	10^{-6}	$A^*(1,\theta)$
$\theta = 0^\circ$	23	71	11	20	36	15	25	7	7	8	5.09098
15°	19	57	10	18	32	9	17	6	7	8	4.93242
30°	17	51	9	17	32	7	9	5	6	7	4.54397
45°	15	49	9	17	31	7	11	5	5	6	4.10228
60°	15	47	9	16	29	5	9	4	5	6	3.72865
75°	17	49	9	17	29	7	13	5	6	7	3.47912
90°	19	57	10	18	32	13	23	6	7	8	3.38875

Numerical values of the abscissae and weights for eight- and 12-term Gauss–Legendre quadratures, calculated using the method given by Press *et al.* (1986), are listed in Table 1.

3. Results of the calculations

First, accurate values of the transmission coefficients $A(\mu R, \theta)$ were evaluated by applying a Gauss–Legendre quadrature of 100 × 100 terms to a modified version of equation (1), where substitution of a variable $x = \sin\omega$ is applied to remove the singularity of the integrand. The accuracy of the values was confirmed by viewing the asymptotic behaviour of the calculated values of the transmission coefficients on increasing the number of terms N. The values of the absorption correction $A^*(\mu R, \theta)$ calculated for $\mu R = 1$ and $\theta = 0, 15, \ldots, 90^\circ$ are listed in the final column of Table 2.

Next, the minimum numbers of terms N necessary to obtain the values of the transmission coefficients within predefined relative errors were searched for by applying the two methods of numerical integration in conjunction with the formulae given by equations (1) and (2). The numbers were determined by detecting five continuing correct values within the allowed errors on increasing the number of terms for the numerical integrals.

Table 2 lists the estimated minimum numbers of terms N needed to obtain the correct value of the transmission coefficient for μR = 1 within the relative allowable errors of $\varepsilon = 10^{-3}$ and 10^{-4} for Simpson's method, and ε = 10^{-4}, 10^{-5} and 10^{-6} for the Gauss–Legendre quadrature. It is clearly seen that the Gauss–Legendre quadrature is more efficient than Simpson's method for both mathematical formulae. Note that the computation time for the two-dimensional numerical integral is roughly proportional to N^2, unless parallel computing is applied. It was also found that the enhanced accuracy of $\varepsilon = 10^{-6}$ is obtained with only a slightly increased computational cost when the formula of equation (2), proposed by Thorkildsen & Larsen (1998*a*,*b*), is applied.

Table 3
Number of terms N needed to obtain the values of the transmission coefficients for μR = 0.5, 1.0, ..., 4.0 within relative errors of $\varepsilon = 10^{-6}$ by applying the Gauss–Legendre quadrature to the formula of Thorkildsen & Larsen.

μR	0.5	1	1.5	2	2.5	3	3.5	4
$\theta = 0^\circ$	8	8	9	10	11	12	12	13
15°	6	8	8	9	10	9	10	11
30°	6	7	7	8	8	9	9	10
45°	6	6	7	7	8	7	8	9
60°	5	6	7	6	7	8	8	8
75°	7	7	8	8	9	9	7	8
90°	7	9	8	10	11	12	12	13

Table 3 lists the minimum number of terms of the Gauss–Legende quadrature needed for the accuracy of ε = 10^{-6}, applied to the formula of Thorkildsen & Larsen, for the values μR = 0.5, 1.0, ..., 4.0 and θ = 0, 15, ..., 90°. Since the formula of Thorkildsen & Larsen reduces to a one-dimensional integral in the limits $\theta \to 0$ and $\pi/2$, it is natural that the two-dimensional numerical integration becomes less effective when θ approaches 0 or $\pi/2$. However, it is not advised to change the formula for different values of θ, because this will make the algorithm more complicated to retain continuity of the calculated values.

The accuracy achieved by the 8 × 8-term Gauss–Legendre quadrature applied to the formula of Thorkildsen & Larsen is better than that of Dwiggins (1975) over the region $0 \le \mu R \le 2.5$. One can easily obtain improved accuracy, simply by increasing the number of terms N.

4. Conclusion

The Gauss–Legendre quadrature applied to the formula proposed by Thorkildsen & Larsen (1998*a*,*b*) provides an efficient numerical method to evaluate transmission coefficients and absorption correction factors for cylinders. Results are obtained for arbitrary values of μR and θ by a simple algorithm for the numerical integrations, without interpolation in a table of numerical values.

References

Dwiggins, C. W. (1975). *Acta Cryst.* A**31**, 146–148.
Maslen, E. N. (1999). *International Tables for Crystallography*, Vol. C, edited by A. J. C. Wilson, pp. 520–529. Dordrecht: Kluwer Academic Publishers.
Press, W. H., Flannery, B. P., Teukolsky, S. A. & Vetterling, W. T. (1986). *Numerical Recipes*. Cambridge University Press.
Thorkildsen, G. & Larsen, H. B. (1998*a*). *Acta Cryst.* A**54**, 172–185.
Thorkildsen, G. & Larsen, H. B. (1998*b*). *Acta Cryst.* A**54**, 186–190.