can be either increased or decreased by simultaneous diffraction, and the extreme values are given in Table 1. For every multibeam case, a particular azimuth φ_0 is computed corresponding to a situation in which one or two reciprocal lattice nodes lie on the Ewald sphere. When the actual azimuth φ differs from φ_0 by more than $\Delta\varphi/2$ as given in Table 1, the 002 integrated intensity is practically restored to the two-beam value.

Table 1 shows that these effects are by no means negligible, especially in the case of the $\bar{1}31$. However, the azimuthal width for the $\bar{1}31$ (14 sec) must be compared with the vertical divergence, *i.e.* perpendicular to the diffraction plane, of the incident beam in Borgonovi & Caglioti's experiment. This vertical divergence amounts to 76 minutes, as calculated from a description of the experimental set up given by Caglioti & Ricci (1962). It is clear, therefore, that only a negligible fraction of the incident beam satisfies the conditions for multiple diffraction. The remaining portion undergoes two-beam 002 diffraction and is totally collected by the counter. The net effect turns out to be of the order of 1·7 % which is within the limits of the experimental error.

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References

Borgonovi, G. & Caglioti, G. (1962). *Nuovo Cim.* **24**, 1174.
Caglioti, G. & Ricci, F. P. (1962). *Nucl. Instr. Methods*, **15**, 155.
Colella, R. (1972). *Acta Cryst.* A**28**, 11.
Colella, R. & Menadue, J. (1972). *Acta Cryst.* A**28**, 16.
Moon, R. M. & Shull, C. G. (1961). *Bull. Amer. Phys. Soc.* **6**, 261.

Acta Cryst. (1972). A**28**, 219

Analytical solution for the X-ray absorption factor for cylinders in two special cases.

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The equation for the absorption factor at Bragg angles of 0 and 90° is integrable, resulting in simple equations that are functions of well-known higher transcendental functions. Numerical results are easily obtained, and a comparison with those obtained using numerical integration is made.

For small-angle scattering studies of cylindrical samples, it is useful to calculate the absorption factor at zero Bragg angle directly, in a manner that does not require a large amount of computer storage. Also, direct calculations at Bragg angles of 0 and 90° allow checks to be made on absorption factors calculated by numerical integration.

The general equation for the transmission factor A that is the reciprocal of the absorption factor A^* is

$$A = \frac{1}{V}\int_V \exp(-\mu L)\,\mathrm{d}V\,, \qquad (1)$$

where V is the sample volume, μ is the linear absorption coefficient, and L is the total path length of the X-ray beam in the sample.

After introducing boundary conditions for the sample shape, transformation of coordinates, and integration by parts, definite integrals, for which solutions are well known, were obtained from equation (1) for Bragg angles of 0 and 90°. The equations for the transmission factors for these two special cases are:

$$A = 2[I_2\{z\} - \mathbf{L}_2\{z\} + (I_1\{z\} - \mathbf{L}_1\{z\})/z - (2z)/(3\pi)] \quad (\theta = 0°) \quad (2)$$

$$= 2[(I_0\{z\} - \mathbf{L}_0\{z\}) - (I_1\{z\} - \mathbf{L}_1\{z\})/z]\,,$$

$$A = [I_1\{2z\} - \mathbf{L}_1\{2z\}]/z\,, \qquad (\theta = 90°) \quad (3)$$

where $z = 2\mu R$, R is the radius of the cylinder, and I_ν and $\mathbf{L}_\nu$ are the modified Bessel function and the modified Struve function respectively of order ν (Erdélyi, Magnus, Oberhettinger & Tricomi, 1953).†

The numerical values of I_ν and $\mathbf{L}_\nu$ can be obtained using series solutions only slightly more complicated than those for the simple transcendental functions, such as the sine. Because series solutions are simple to evaluate on a computer, it is quite simple to solve for the absorption correction directly for the two special cases.

For large values of the arguments of the modified Bessel and Struve functions, these functions become very large,

Table 1. *Values of A^**

	$\theta = 0°$		$\theta = 90°$	
μR	A^*	% Error‡	A^*	% Error
0·5	2·300	0·43	2·050	0.01
1·0	5·091	0·61	3·389	0·04
1·5	10·75	0·45	4·863	0·15
2·0	21·44	0·63	6·389	0·17
2·5	40·10	0·74	7·936	0·30
3·0	70·12	0·88	9·492	0·40
4·0	177·0	1·11	12·62	0·66
5·0	363·0	1·11	15·75	0·97

‡ Percent error in A^* values in *International Tables for X-ray Crystallography* (1959) when compared with A^* values given in this table.

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† Proofs of equations (2) and (3) are available from the author.

and many significant figures are lost when they are combined as indicated in equations (2) and (3). Thus, a double-precision computer program should be used, and π should include the maximum allowed number of significant figures. For a computer allowing a maximum of 16 significant figures, μR may be as high as 5, if a precision of at least four significant figures is desired in A^*.

Values of the absorption factor are given in Table 1, and these values are compared with those in *International Tables for X-ray Crystallography* (1959), that were obtained by numerical integration. Agreement is good at lower values of μR, but a small amount of error becomes apparent in the values obtained by numerical integration at higher values of μR.

Values of the absorption factor at higher values of μR could be calculated using asymptotic expressions for I_ν–L_ν. This was not done because the values of μR used were of sufficient range for most purposes. If a very large value of μR is encountered, it is best either to reduce the radius of the sample or to use shorter wavelength radiation to reduce μR, because the change of the absorption factor with scattering angle becomes huge near 0° for large μR, and only small deviations of the sample shape from that used for the calculations can produce large errors.

Also, secondary scattering is likely to be quite important for large values of μR when the sample is noncrystalline.

Equations (2) and (3) can be solved at several values of z without a computer, using values of I_ν–L_ν given in the *Handbook of Mathematical Functions* (1964). Interpolation between values obtained will give results of sufficient accuracy for most purposes.

References

ERDÉLYI, A., MAGNUS, W., OBERHETTINGER, F. & TRICOMI, F. G. (1953). *Higher Transcendental Functions*, Bateman Manuscript Project. California Institute of Technology, Vol. 2, Ch. VII. New York: McGraw-Hill.

Handbook of Mathematical Functions (1964). National Bureau of Standards **AMS 55**, 2nd. printing. Washington, D.C.: U.S. Government Printing Office.

International Tables for X-ray Crystallography (1959). Vol. II. Birmingham: Kynoch Press.

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Out-of-zone effects in dynamic electron diffraction intensites from gold. Erratum.

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Corrected labelling is given for Fig. 11 in *Acta Cryst.* (1971) A**27**, 399.

In Fig. 11 of the article by Lynch (1971) the labelling of the four parts was printed incorrectly. The letters (*a*), (*b*), (*c*), (*d*) should be (*d*), (*c*), (*b*), (*a*) respectively, reading from top to bottom of the diagram.

Reference

LYNCH, D. F. (1971). *Acta Cryst.* A**27**, 399.

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The mean figure-of-merit for a difference Fourier synthesis.

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The conventional difference Fourier synthesis has a mean figure-of-merit of $(2/\pi)$ times that of the native structure, and has coefficients which are correctly weighted for the 'best' synthesis of Blow & Crick [*Acta Cryst.* (1959) **12**, 794].

Workers in protein structure analysis commonly use difference Fourier syntheses with coefficients:

$$m_P\mathbf{F_D} = m_P(F_H - F_P)\exp{(i\varphi_P)}\,. \qquad (1)$$

Here, F_P and φ_P are the amplitude and phase of a structure factor of the native crystal, and F_H is the amplitude of the same structure factor of a slightly modified crystal. The figure-of-merit m_P is discussed later on. Typically, these syntheses are used not for refinement but to reveal the details of small additions or alterations to the native structure. It may then be useful to calculate the accuracy of such difference syntheses in the same framework used for assessing conventional protein structure determinations.

Blow & Crick (1959) show that, in a least-squares sense, the 'best' Fourier synthesis has coefficients in which the observed amplitudes are weighted by a figure-of-merit that is given approximately by the cosine of the expected error in the phase angle. The quantity m_P in equation (1) is, therefore, the cosine of the error in φ_P.

Fig. 1 shows the structure factors $\mathbf{F_P}$ and $\mathbf{F_H}$, as well as the correct difference structure factor $\mathbf{f_D}$ to which $\mathbf{F_D}$ is an approximation. The phase error in the coefficient