

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  $\pi$  should include the maximum allowed number of significant figures. For a computer allowing a maximum of 16 significant figures,  $\mu R$  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  $\mu R$ , but a small amount of error becomes apparent in the values obtained by numerical integration at higher values of  $\mu R$ .

Values of the absorption factor at higher values of  $\mu R$  could be calculated using asymptotic expressions for  $I_v-L_v$ . This was not done because the values of  $\mu R$  used were of sufficient range for most purposes. If a very large value of  $\mu R$  is encountered, it is best either to reduce the radius of the sample or to use shorter wavelength radiation to reduce  $\mu R$ , because the change of the absorption factor with scatter-

ing angle becomes huge near  $0^\circ$  for large  $\mu R$ , 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  $\mu R$  when the sample is noncrystalline.

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

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

*Acta Cryst.* (1972). A28, 220

**Out-of-zone effects in dynamic electron diffraction intensities from gold. Erratum.** By D. F. LYNCH, *Division of Chemical Physics, CSIRO, P.O.Box 160, Clayton 3168, Australia*

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Corrected labelling is given for Fig. 11 in *Acta Cryst.* (1971) A27, 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.* A27, 399.

*Acta Cryst.* (1972). A 28, 220

**The mean figure-of-merit for a difference Fourier synthesis.** By EATON E. LATTMAN, *Department of Biophysics, Johns Hopkins University, Baltimore, Maryland 21218, U.S.A.*

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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 incorrectly 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:

$$m_p \mathbf{F}_D = m_p (F_H - F_p) \exp(i\varphi_p). \quad (1)$$

Here,  $F_p$  and  $\varphi_p$  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  $\varphi_p$ .

Fig. 1 shows the structure factors  $F_p$  and  $F_H$ , 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

$F_D \exp(i\varphi_P)$  is  $(\varphi_P - \varphi_D)$ , and so the correctly weighted amplitude is  $f_D \cos(\varphi_P - \varphi_D)$ . Since  $f_D$  is generally small compared with  $F_P$  or  $F_H$ , it is clear from Fig. 1 that  $F_D = F_H - F_P \simeq f_D \cos(\varphi_P - \varphi_D)$ , and is, therefore, the correctly weighted amplitude for the phase discrepancy  $(\varphi_P - \varphi_D)$ .

The error in  $\varphi_P$  itself is accounted for by the factor  $m_P$ . The two phase errors are approximately independent, so that in the difference synthesis the figure-of-merit,  $m_D$ , for a reflection is given approximately by  $m_P \cos(\varphi_P - \varphi_D)$ . The mean figure-of-merit for all reflections is given by

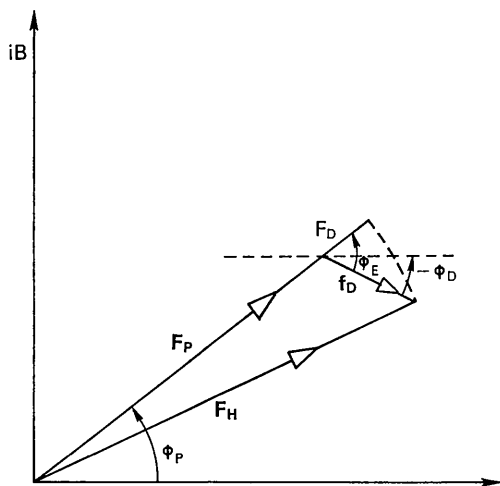


Fig. 1.  $F_P = F_P \exp(i\varphi_P)$  is a structure factor for the native crystal and  $F_H = F_H \exp(i\varphi_H)$  is the corresponding structure factor for this crystal slightly modified. The vectorial difference between them is  $f_D = f_D \exp(i\varphi_D)$ ;  $f_D$  is, therefore, the correct difference coefficient.  $F_D = |F_H - F_P|$  is the amplitude of the approximate difference coefficient, and  $\varphi_E = \varphi_P - \varphi_D$  is the difference between the phase of the correct and approximate coefficients.

$$\langle m_D \rangle = \langle m_P \rangle \langle \cos(\varphi_P - \varphi_D) \rangle. \quad (2)$$

The phase  $\varphi_D$  is *random* with respect to  $\varphi_P$ . Taking account of the sign of  $(F_H - F_P)$  the phase discrepancy is seen to be uniformly distributed in the interval  $(-\pi/2, \pi/2)$ . The mean value of the cosine over this interval is  $2/\pi$ , so that

$$\langle m_D \rangle = \langle m_P \rangle (2/\pi). \quad (3)$$

The quantity  $\langle m_P \rangle$  is, of course, usually known from the structure analysis of the native material.

The root-mean-square error in an electron density function is related to the mean figure-of-merit through a formula given by Dickerson, Kendrew & Strandberg (1961). The relation depends on the assumption that errors in the coefficient amplitudes are small compared to errors in the phases, and is, therefore, of dubious validity for difference synthesis in which amplitude errors are large. A complete error analysis of the difference synthesis is, therefore, still lacking.

In summary, it has been shown that a difference Fourier synthesis calculated using  $m_P(F_H - F_P) \cdot \exp(i\varphi_P)$  as coefficients has a mean figure-of-merit of  $(2/\pi) \cdot \langle m_P \rangle$ , and is correctly weighted in the sense of Blow and Crick.

I should like to thank Dr Max Perutz for his helpful comments.

*Note added in proof:* a very complete analysis of errors in the difference Fourier technique has recently been given by Henderson & Moffat (1971).

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 DICKERSON, R. E., KENDREW, J. C. & STRANDBERG, B. E. (1961). *Acta Cryst.* **14**, 1188.  
 HENDERSON, R. & MOFFAT, J. K. (1971). *Acta Cryst.* **B27**, 1414.

#### Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.*

**An introduction to crystallography.** By W. KLEBER. Pp. 366. Berlin: Veb-Verlag Technik, 1971. Price Dm 36,00.

The original *Einführung in die Kristallographie* first appeared in 1956 and its popularity is demonstrated by the fact that the German edition currently in print is the tenth; the book under review is a translation by W.A. and A. M. Wooster of this tenth German edition. It is very sad to record that Professor Kleber died in 1970 without having seen the first English edition.

The title *Introduction to Crystallography* – which incidentally has already been used by more than one author – could be interpreted in many ways; it could deal with anything from the purely formal elements of classification and symmetry to modern developments in crystal optics or in crystal chemistry. It is unusual to find a single book such

as Professor Kleber's which manages to combine successfully a considerable amount of classical theory and, at the same time, many up-to-date applications.

The secret is undoubtedly in the author's attitude to his subject. In the very first words of the introduction Professor Kleber points out that, while physics and chemistry are concerned with processes and changes, crystallography – in common with mineralogy, botany, zoology, etc. – is more concerned with the study of a specific object, in this case, a crystal. It is thus possible to include, quite logically, in a single volume, not only a very careful and precise section (about 90 pages) on the basic theory of crystal structure, starting from the laws derived from measurements of external morphology, dealing systematically with all the various symmetry operations and in considerable detail with the 32 crystal classes, but also with sections of similar length on crystal chemistry and on crystal physics and a