

The Determination of Structure Factors From Dynamical Effects in Electron Diffraction

By J. M. COWLEY

School of Physics, University of Melbourne, Parkville, Victoria 3052, Australia

In order to obtain accurate data on structure factors from electron diffraction data, it is necessary to take into account the inevitable n -beam dynamical diffraction effects. The comparison of intensity values from detailed computer calculations with observed intensities from perfect crystals is reviewed for the cases of convergent beam diffraction patterns from MgO crystals of uniform thickness and of dark-field images of wedge-shaped crystals of silicon. An analysis of the sources of error in each case suggests that it may be possible to derive structure factor values with an accuracy of better than one per cent. The method, recently proposed by Watanabe *et al.* [*Acta Cryst.* (1968). A 24, 249] for deriving structure factors from the values of accelerating voltages for which some Kikuchi lines disappear, is reviewed and possible sources of error are examined.

Introduction

The derivation of structural information on crystals from electron diffraction data differs from that for the X-ray case in several important respects. One is that the information refers to the potential distribution rather than the electron density distribution. This produces no significant differences in the positions found for the centres of any but the lightest of atoms, but may lead to appreciable differences in the details of the distributions associated with the ionization, bonding and thermal motions of atoms. As will be shown later, conversion to data in electron density distributions is possible and may, within certain limitations, be simple.

Of greater practical importance is the almost universal occurrence of dynamical diffraction effects which cannot be adequately described in terms of the two-beam approximation, usual in X-ray diffraction, when any degree of precision is required. The number of coherently-interacting simultaneously-diffracted beams which must be taken into account to give an accurate representation of intensities varies from ten to fifty or more, depending on the experimental conditions.

The case for which a simple kinematical approximation is most nearly valid is that of the ring or arc patterns, given by polycrystalline materials, such as are used for structure analysis by the workers in the Soviet Union (Vainshtein, 1964). For many samples, corrections have been made to intensities by means of Blackman's (1939) two-beam theory for powder patterns. However it has recently been shown (Turner & Cowley, in preparation) that, even when tests based on the two-beam approximation indicate no appreciable dynamical effects, n -beam interactions may provide significant modifications of the intensities and so limit the accuracy of a structure analysis. It may be that, when an adequate account of n -beam interactions can be incorporated in the interpretations of intensities, it will be possible to obtain high accuracy in structure analysis based on such data, but this has not yet been achieved. A

review of the present situation is given by Cowley (1967).

Dynamical diffraction effects obtained with single-crystal specimens were detected and recognized many years ago in electron diffraction work. MacGillavry (1940) explained details of convergent beam diffraction patterns of mica and used them to derive structure factors by means of a two-beam approximation. The same approximation was used with reasonable success by Heidenreich & Sturkey (1945) to explain Pendelösung fringes observed in electron microscope images of wedge-shaped fringes and by Sturkey (1948) to explain the fine-structure splitting of diffraction spots given by crystals of regular shape.

However recent observations and calculations have indicated that, for each of these types of experiment, the two-beam approximation gives results which are in error by five to ten per cent in even the most favourable circumstances. In order to approach the degree of accuracy which is now regarded as significant for providing structural information on the relatively simple substances so far involved, it is necessary to work entirely in terms of n -beam dynamical theory and computations.

The calculation of n -beam intensities

The introduction of suitable programs for moderate to large size computers has now provided the possibility of routine calculation of the intensities of diffracted beams given by perfect crystals with arbitrary accuracy. Calculations for imperfect crystals are necessarily more difficult but considerable progress is being made in this direction also. Calculations are made using either the slice method, developed by Goodman & Moodie (1965) on the basis of the slice-formulation due to Cowley & Moodie (1957) and reviewed by Cowley (1967), or the matrix method (Howie & Whelan, 1961; Fisher, 1968). The computing times, convenience and accuracy of these two methods are comparable for medium-size computers. From the considerable number of calculations already made, some general conclusions can be drawn.

For the incident beam near to a principal orientation, a two-dimensional spot pattern is produced and about fifty beams must be considered for even the simplest of structures. The variations of diffracted beam intensities with crystal thickness and orientation are very complicated except for the most symmetrical of conditions (Fisher, 1968).

The simplest cases, involving the smallest numbers of beams, are those given for carefully chosen orientations of the crystal such that only a single row of diffraction spots, passing through the origin, is excited with appreciable intensity. Such cases involve only the 'systematic interactions' between the various orders of reflexion from a set of lattice planes. When the incident beam satisfies the Bragg angle for the strong innermost reflexion of such a row for a simple structure with light atoms, we have the closest approach to purely 'two-beam' conditions. Calculations show that even for these conditions the Pendellösung periodicity or 'extinction distance' is modified by five to ten per cent by the presence of the weaker beams (Hirsch, Howie, Nicholson, Pashley & Whelan, 1965; Goodman & Lehmpfuhl, 1967).

If no absorption is included in the calculations, there is no convergence towards a two-beam situation with increasing crystal thickness. All beam intensities oscillate strongly but the strong and weak beams maintain, on the average, the same relative intensities. If absorption is introduced there is a very slow concentration of energy in the two strongest beams for large thicknesses for some crystals, but a divergence from the two-beam situation for other crystals (Fisher, in preparation).

The intensities of the diffracted beams depend not only on the crystal thickness and orientation but are also very sensitive to the absolute amplitudes and relative phases of the structure factors. This leads to the possibility of deriving accurate structure factor values from observations on crystals for which the crystal perfection can be ensured and the morphology and orientation can be adequately defined. Since the region of crystal needed to provide the diffraction observations may have dimensions of about one micron or, often, very much less, the requirement of crystal perfection is relatively easily met. Developments of both the convergent beam diffraction technique and the observation of thickness fringes may provide adequate control of the other experimental variables and have been explored as a basis for structure factor determinations. Further investigations of the refraction splitting of diffraction spots have recently revealed interesting effects of n -beam interactions (Lehmpfuhl, private communication) but the prospect for deriving accurate structural data in this way seems more remote.

Convergent beam diffraction experiments

The techniques now used for obtaining convergent beam diffraction patterns from very small areas (500 Å or less in diameter) of parallel-faced, perfect crystals

have been described by Goodman & Lehmpfuhl (1964) and Cockayne, Goodman, Mills & Moodie (1967). The method provides a record of the variation of the intensities of all diffracted beams with the angle of incidence of the primary beam, for constant crystal thickness. Corresponding calculations are made on the basis of assumed values for the Fourier coefficients of the potential distribution, and these coefficients are varied to obtain the best possible fit with the observations.

The crystal thickness is determined at first roughly by observations on the shape-transform detail of intensity distributions for weak reflexions and then is refined as a parameter of the calculations. An accuracy of better than one per cent is obtainable. Some allowances must be made for thermal motions of the atoms and for absorption effects, but for the former an elementary treatment using X-ray Debye-Waller factors is usually adequate, and absorption has very little effect except on the primary beam.

A detailed study on MgO has been made by Goodman & Lehmpfuhl (1967) using the $h00$ line of systematic reflexions from perfect flat crystals, of about 500 Å thickness, tilted to one of the two orientations which provide almost complete absence of non-systematic interactions. They derived a temperature-corrected value for the 200 Fourier coefficient of $V_{200} = 7.02$ volts. This compared well with values derived from the most recent calculations of MgO, which give potentials ranging from 6.90 to 7.27 volts. From the sensitivity of the calculated dependence of intensity on angle to changes in the assumed values of these structure factors and an analysis of possible experimental errors, an accuracy of better than one per cent seemed possible.

A further study of the situation has revealed that, even for the orientations carefully chosen to minimize the effect of non-systematic interactions, the intensities given by their one-dimensional calculations, involving systematic $h00$ interactions only, are not exactly the same as those given by the full two-dimensional calculations for the same orientations. But the inclusion of the non-systematic interactions does not change the value of the 200 structure factor giving best fit with the experimental intensities. However, full two-dimensional calculations, made for other, less favourable orientations, taking into account all possible non-systematic interactions, have shown errors in structure factors deduced from the one-dimensional calculations amounting to two or three per cent. It is therefore important that the additional difficulties and more laborious procedures of two-dimensional computation should be undertaken, at least to check representative cases, when one-dimensional calculations are used for the refinement of structure factors. (P. Goodman & A. G. McMahon, private communication).

Thickness fringes in electron micrographs

The bright field image of a wedge-shaped crystal, obtained with the primary transmitted beam, and the set

of dark-field images obtained using the various diffracted beams provide an immediate measure of the variation of the diffracted intensities with crystal thickness. Since the available computing methods provide intensities as a function of crystal thickness most readily, a single 'run' on the computer gives the data for comparison with an experiment, provided that the crystal orientation, electron wavelength and other experimental factors are adequately determined.

Normal dark-field images, obtained by translating the objective aperture, suffer from loss of resolution and contrast because electrons which lose energy in the specimen are displaced in the image by the strong off-axis chromatic aberration of the objective lens. It is preferable to use the high-resolution dark-field technique of tilting the beam incident on the specimen so that the diffracted beams are made axial. The principle of reciprocity ensures that the diffracted intensities will be the same as in aberration-free 'normal' dark field images (Pogany & Turner, 1968).

In order to reduce the requirements for microscope resolution, it is convenient to spread the thickness fringes by using a relatively small-angle crystal wedge. For initial experiments therefore, thin wedges of silicon (wedge angle around 30°), obtained by shattering large crystals, were employed instead of the 90° wedges of MgO traditionally used for thickness-fringe observations.

The orientations of the crystals were obtained with sufficient accuracy from Kikuchi-line patterns, which could also be used for accurate determinations of electron wavelength.

For a strictly two-beam case, with the Bragg angle satisfied, the Pendellösung periodicity depends on the single parameter of the structure factor for the one reflexion, and a knowledge of the wedge angle is necessary in order to determine this periodicity from the thickness fringes. For n -beam cases, however, the intensity variations depend not only on the structure factors but also on the excitation errors which are determined by the incident beam direction and the wavelength. Then the structure factors may be derived on an absolute basis by comparison with the excitation errors, and no knowledge of the wedge angle or of the electron microscope magnification is necessary.

Experience has shown that silicon wedges formed by fracture usually have accurately flat faces, so that there is a linear relationship between distance from the crystal edge and crystal thickness and no detailed calibration of crystal thickness is necessary.

Pollard & Turner (in preparation) have proposed a 'turning-point analysis' for the initial stages of refinement of structure factors. In this the positions of maxima and minima of the experimental and calculated intensity curves are compared for various diffracted beams and various incident beam orientations. Thereby, uncertainties in intensities created by difficulties in subtracting background from the experimental curve are avoided. But, for greatest accuracy, the detailed

variations of intensity with thickness must presumably be used and for this purpose the subtraction of inelastically scattered electrons by energy analysis will be valuable.

Pollard has made detailed calculations on the effect of variation of the 111 and 222 structure factors for silicon in an attempt to confirm or refine the conclusions regarding the distribution of bonding electrons obtained from X-ray diffraction data by Dawson (1967).

In Fig. 1, the observed intensity variation is compared with curves calculated for several different assumed values of the structure factors for the case of the 222 reflexion with the incident beam at the Bragg angle for the 111 [Fig. 1(a)] and 222 [Fig. 1(b)] reflexions. The best agreement with experiment was found for values of f_A , the part of the structure factor due to one atom (Dawson, 1967), of about $f_A(111) = 3 \cdot 10 \text{ \AA}$ and $f_A(222) = 0 \cdot 002 \text{ \AA}$; considerably different from the values $f_A(111) = 2 \cdot 83$ and $f_A(222) = 0 \cdot 047$ which correspond to Dawson's deductions from X-ray results and also from the values $f_A(111) = 3 \cdot 248$ and $f_A(222) = 0$, obtained using the relativistic Hartree-Fock potentials for isolated neutral atoms (Doyle & Turner, 1968).

However, as in the case of the convergent beam experiments on MgO, these initial results are based on one-dimensional calculations of systematic interactions only, and it is possible that the full two-dimensional calculations now in progress may give more accurate results differing from these by one or two per cent of the $f_A(111)$ value.

The fitting of calculated to experimental intensity curves for both the wedge method and the convergent beam diffraction method depends at the moment on a trial-and-error procedure. Although the calculations can be made quite rapidly with available computers, this is still rather cumbersome, and a systematic refinement procedure would be of considerable value.

The disappearance of Kikuchi lines

Recently an entirely new basis has been proposed for the derivation of accurate structure factor values. This derives from the observation (Uyeda, 1968) that particular members of the set of parallel Kikuchi lines, due to the various orders of reflexion from one set of planes, appear to vanish for particular values of the electron accelerating voltage in the high-energy, relativistic, region (greater than about 200 keV). Watanabe, Uyeda & Kogiso (1968) have interpreted such extinctions in terms of zero values for the effective structure factor values, U'_h , derived from Bethe's second approximation (Bethe, 1928), the so-called 'Bethe potentials'.

When the excitation error, ζ_h , is zero, as at the Kikuchi line position for the h reflexion, these may be written (Uyeda, 1968):

$$U'(h) = R \left[U(h) - Rd^2 \sum_{h_1} \frac{U(h_1)U(h-h_1)}{h_1(h-h_1)} \right], \quad (1)$$

where $U(h) = (2me/h^2)V(h)$, d is the interplanar spacing for the first order reflexion and R is the relativistic factor given by $R = (1 + eE/mc^2)$. The values of R required to make $U'(h)$ equal to zero for some second-order reflexions from simple metallic structures correspond to voltages, E , in the range 300 to 400 keV and agree well with the voltages for which the corresponding Kikuchi line extinctions are observed.

If the right hand side of equation (1) is put equal to zero, we have a relationship between structure factors. Then, for example, the first-order structure factor, U_1 , may be determined in terms of the structure factors for higher orders which are more accurately known because their dependence on the configuration of the outer bonding electrons is much smaller.

In this way Watanabe, Uyeda & Fukuhara (1968) have derived electron structure factors and hence values for X-ray atomic scattering factors, for the 110 reflexion of Fe and the 111 reflexion of Ni and Al, which are in good agreement with other available results. The relevant experimental parameters are deter-

mined with good accuracy, leading to errors of less than one per cent. The validity of the Bethe second approximation was tested by n -beam calculations, made using the matrix method of Fukuhara (1966). The accuracy with which equation (1) gives the correct zeros was found to be very good, so that the resulting errors in the derived $U(h)$ values amount to less than 0.1%.

A partial explanation for this rather surprising indication of accuracy for the Bethe approximation is provided by considerations of the n -beam theory appropriate to Kikuchi lines. For thick crystals the electrons forming the Kikuchi lines have undergone, on the average, a large number of elastic and inelastic scattering processes, so that the Kikuchi line intensity may be considered as given by the incoherent addition of electron beams originating from various depths in the crystal. Thus, to a good approximation,

$$I(h) = \int_0^{\infty} |T_1(h) + T_2(h) + T_3(h) + \dots|^2 dH, \quad (2)$$

where H is the crystal thickness and T_1, T_2, \dots etc.

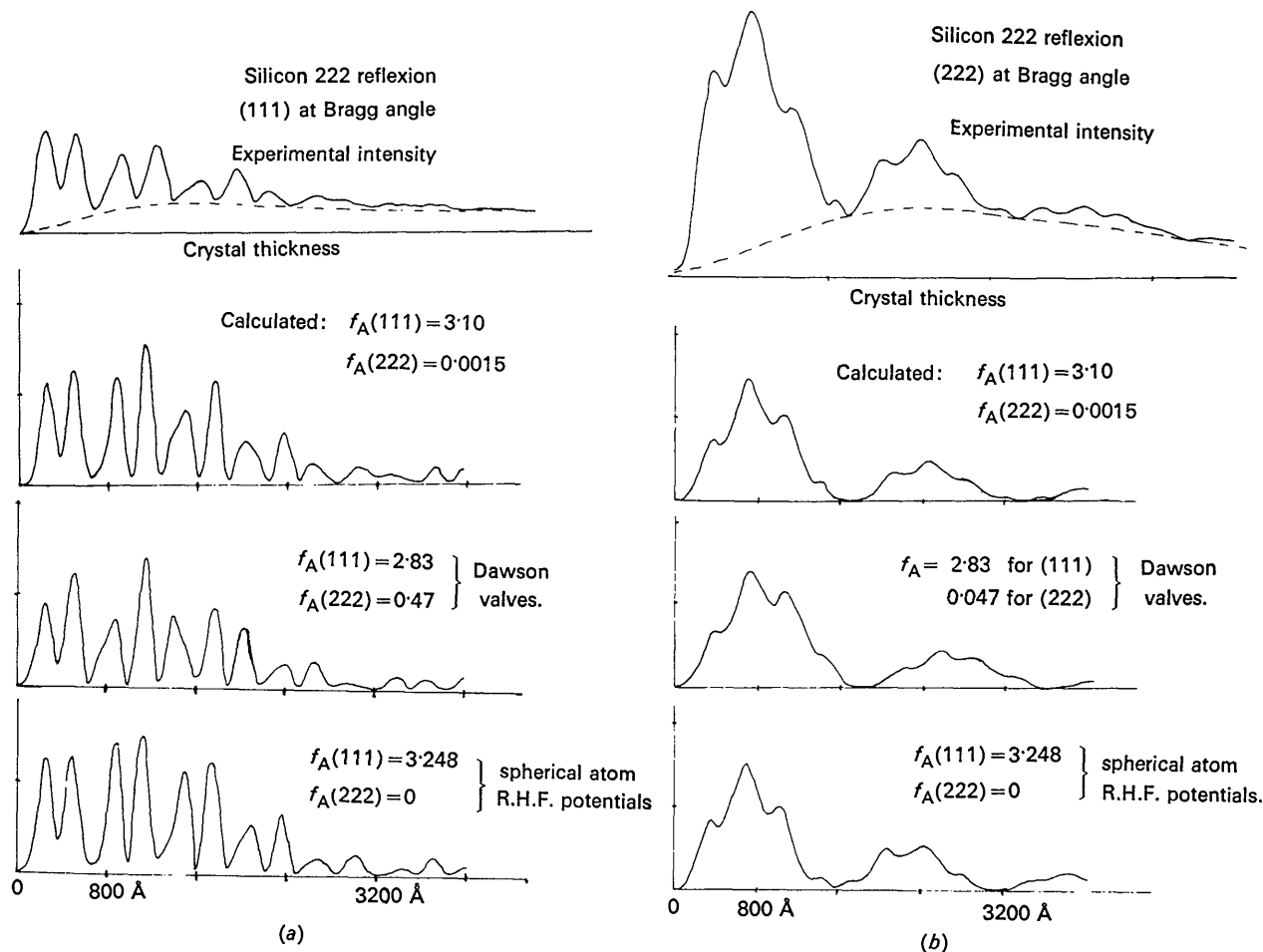


Fig. 1. (a) Comparison of observed and calculated intensity of the 222 reflexion from silicon with the Bragg condition satisfied for the 111 reflexion. The experimental curve was obtained by microdensitometer measurement of the dark field electron microscope image. (b) As for (a), but with the 222 Bragg condition satisfied.

represent the contributions of beams scattered once, twice and so on, *i.e.* the terms of the Born series development for n -beam diffraction in a crystal. Making use of the expressions for T_n derived by Cowley & Moodie (1957) it can be shown (Cowley, in preparation) that, for $\zeta_h=0$, equation (2) gives

$$I(h) = \frac{R^2 \pi^2 \lambda^2}{4\mu_0^3} \left| U(h) - Rd^2 \sum_{h_1} \frac{U(h_1)U(h-h_1)}{h_1(h-h_1)} + R^2 d^4 \right. \\ \left. \times \sum_{h_1} \sum_{h_2} \frac{U(h_1)U(h_2)U(h-h_1-h_2)}{h_1(h-h_1)(h_1+h_2)(h-h_1-h_2)} - \dots \right|^2. \quad (3)$$

The first two terms of the series included here are identical with (1). It does not follow, however, that if the sum of the first two terms is zero, the sum of the whole series will be zero. In fact alternate terms in the series will be equal and opposite in sign if

$$U(h-h_{n-1}) = Rd^2 \sum_{h_n} \frac{U(h_n-h_{n-1})U(h-h_n)}{h_n(h-h_n)}, \quad (4)$$

for all h_{n-1} values. Then the special case $h_{n-1}=0$ gives the zero for the sum of the first two terms. It seems unlikely that the general condition (4) can be realized, except for some sort of averaging over the h_{n-1} values which may possibly depend on a favourable relationship between the $U(h_n)$. Thus the generality of agreement between the Bethe potential zeros and those calculated by n -beam methods needs to be justified in detail by further investigations.

Another aspect of the method which requires further study is the possibility that errors are introduced by limiting the calculation of both the Bethe potentials and the n -beam matrix results to the systematic interactions of a one-dimensional set of reflexions. The situation is not so clearly defined as for the convergent beam or wedge crystal methods since the disappearance of a Kikuchi line is presumably judged by observing its whole length, corresponding to a variety of orientations of the diffracted beams with respect to the crystal.

Conclusions

It is apparent from the above that the methods for the derivation of accurate structure factor values from dynamical effects in electron diffraction are in a relatively early stage of development. The sources of error and considerations of accuracy are, for the most part, entirely different from those met in X-ray diffraction methods, but the present understanding of n -beam diffraction effects is sufficient to justify claims that present results are certainly accurate to within a few per cent. Tests and refinements of the methods, now in hand, should ensure an error of less than one per cent. One remaining factor of uncertainty in the interpretation of the results comes from the fact that absorption effects add a small real part as well as an imaginary part, to the effective potentials. This probably does not affect the present results seriously, but should be evaluated in detail in the future.

A further possible method for obtaining accurate data on structure factors, as yet untested, arises from the possibility that, after integration over crystal thickness, zeros of intensity may be obtained for some reflexions when the angle of incidence of the primary beam, rather than the accelerating voltage is varied. For this case the Bethe potential approximation is not valid, and no zeros are given by integrations such as equation (2). However it has been shown (Cowley, in preparation) that some zero or minimum values of intensity may be given by a coherent integration of amplitudes over thickness, such as would be appropriate for diffraction from wedge-shaped crystals with well-collimated electron beams.

The primary data obtained from the electron diffraction experiments are values for the Fourier coefficients of the potential distribution. The relation to X-ray diffraction structure factors is provided by Poisson's equation. If the potential distribution can be separated into additive contributions from individual atoms, X-ray scattering factors may be derived from the Mott formula

$$f_{el} = \frac{m_0 e^2}{2h^2} \frac{(Z - f_x)}{s^2},$$

where $s = (\sin \theta)/\lambda$.

However, it should be pointed out that the potential distribution depends on both the electron distribution and the positions of the atomic nuclei, and so contains in principle, some information in addition to that derivable from X-ray data. Any differences in position or thermal vibration of the nuclei and the electron clouds will be reflected in the electron diffraction data. Observable effects of this type may be present, even at the present levels of accuracy, in the case of hydrogen or other light atoms. Hence, conversion to the equivalent X-ray scattering factors should not be automatic. Data on potential distributions should be preserved as such for future reference if not for immediate interpretation.

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References

- BETHE, H. A. (1928). *Ann. Phys. Lpz.* **87**, 55.
- BLACKMAN, M. (1939). *Proc. Roy. Soc. A* **173**, 68.
- COCKAYNE, D. J. H., GOODMAN, P., MILLS, J. C. & MOODIE, A. F. (1967). *Rev. Sci. Instrum.* **38**, 1093.
- COWLEY, J. M. (1967). *Progress in Materials Science*, **13**, No. 6, 269.

- COWLEY, J. M. & MOODIE, A. F. (1957). *Acta Cryst.* **10**, 609.
- DAWSON, B. (1967). *Proc. Roy. Soc. A* **298**, 255, 379.
- DOYLE, P. A. & TURNER, P. S. (1968). *Acta Cryst.* **A 24**, 390.
- FISHER, P. M. J. (1968). *Jap. J. Appl. Phys.* **7**, 191.
- FUKUHARA, A. (1966). *J. Phys. Soc. Japan*, **21**, 2645.
- GOODMAN, P. & LEHMPFUHL, G. (1964). *Z. Naturf.* **19a**, 818.
- GOODMAN, P. & LEHMPFUHL, G. (1967). *Acta Cryst.* **22**, 14.
- GOODMAN, P. & MOODIE, A. F. (1965). Papers in International Conference on Electron Diffraction and Defects in Crystals, Melbourne.
- HEIDENREICH, R. D. & STURKEY, L. (1945). *J. Appl. Phys.* **16**, 97.
- HIRSCH, P. B., HOWIE, A., NICHOLSON, R. B., PASHLEY, D. W. & WHELAN, M. J. (1965). *Electron Microscopy of Thin Crystals*. London: Butterworths.
- HOWIE, A. & WHELAN, M. J. (1961). *Proc. Roy. Soc. A* **263**, 217.
- MACGILLAVRY, C. H. (1940). *Physica*, **7**, 329.
- POGANY, A. P. & TURNER, P. S. (1968). *Acta Cryst.* **A 24**, 103.
- STURKEY, L. (1948). *Phys. Rev.* **73**, 183.
- UYEDA, R. (1968). *Acta Cryst.* **A 24**, 175.
- VAINSHTEIN, B. K. (1964). *Structure Analysis by Electron Diffraction*. Oxford: Pergamon Press.
- WATANABE, D., UYEDA, R. & KOGISO, M. (1968). *Acta Cryst.* **A 24**, 249.
- WATANABE, D., UYEDA, R. & FUKUHARA, A. (1968). *Acta Cryst.* **A 24**, 580.

Acta Cryst. (1969). **A 25**, 134

D2·4

An Accurate Absolute Scattering Factor for Silicon

BY M. HART AND A. D. MILNE

H. H. Wills Physics Laboratory, University of Bristol, Bristol, England

The 220 Bragg reflexion of silicon has been studied in considerable detail. By the Pendellösung fringe method we have measured the atomic scattering factor with an internal consistency of better than 0·1%. Particular care was taken to exclude systematic errors which might arise from elastic strain, X-ray absorption and X-ray polarization effects. The crystal was cut parallel to the Bragg planes at the points of observation so that its thickness could be directly measured with a travelling microscope. At the value of $\sin \theta/\lambda$ corresponding to the 220 Bragg reflexion, the experimental atomic scattering factors (at 20°C) were: $f = 8\cdot478 \pm 0\cdot008$ for Mo $K\alpha_1$ radiation; $f = 8\cdot448 \pm 0\cdot012$ for Ag $K\alpha_1$ radiation, and $f(\text{Mo } K\alpha_1)/f(\text{Ag } K\alpha_1) = 1\cdot0035 \pm 0\cdot0007$.

Introduction

Several authors have recently made measurements of X-ray structure factors by the Pendellösung method (Kato & Lang, 1959; Hattori, Kuriyama, Katagawa & Kato, 1965; Hart, 1966; Hattori & Kato, 1966; Kato & Tanemura, 1967; Yamamoto & Kato, 1968; Batterman & Patel, 1968). However, none of those authors were able to obtain absolute values of structure factors to better than 1%, even on favourable materials such as silicon. In the present measurements on the 220 Bragg reflexion from silicon, we have obtained values of structure factors with deviations of less than 0·1% between separate experiments. Since this is the highest precision ever claimed for a structure factor measurement, we will describe the experimental technique in some detail.

Such precision of course finds immediate applications in studies of the electron distribution in crystals, in discussions of the relative merits of the various theoretical models by which atomic scattering factors are calculated and in the evaluation of possible sources of systematic error in the more conventional techniques by which structure factors are measured. In this con-

text it may be important to notice that the Pendellösung method involves only the coherent part of the X-ray scattering amplitude.

Theory

The spherical wave theory of diffraction by highly perfect crystals has been thoroughly developed in a series of papers by Kato (1960, 1961*a, b*, 1968*a, b*). In addition, the influence on Pendellösung fringes of crystal imperfections, including elastic strains, has been investigated both theoretically (Kato, 1964) and experimentally (Hart, 1966) in considerable detail.

In the symmetric Laue case, with which we are exclusively concerned, the intensity field I_h of the Bragg reflected waves in the spherical wave case of a section pattern (Kato & Lang, 1959) is

$$I_h = A\pi^2 A_0^{-2} \text{cosec}^2\theta \{J_0(\pi q A_0^{-1})\}^2, \quad (1)$$

where A is a constant and θ is the Bragg angle. J_0 is the zero order Bessel function and q is the depth in the crystal measured along the net plane from the X-ray entrance surface (we are concerned only with