In terms of the crystal axes a, b, c it is possible to define reciprocal lattice axes a^*, b^*, c^* in the usual manner. If ξ, η, ζ represent variables along the a^*, b^*, c^* axes respectively, the interference function can be expressed in terms of these quantities. Warren has shown that with the particular choice of axes used, only the z displacement causes a broadening of the reciprocal lattice spot in the c^* direction. On integrating the interference function with respect to ξ, and η, the functional dependence on ζ only is obtained. Warren derived the following equation for this case.

$$I_0(\zeta) = N \sum_{n=0}^{\infty} A_n \cos 2\pi n\zeta + B_n \sin 2\pi n\zeta \, , \tag{3}$$

where ζ is defined so that ζc^* represents a distance along the c^* axis from the (h, k, l) reciprocal lattice point, and

$$A_o = N_3 \tag{4}$$

$$A_n = 2 \sum_{w=0}^{N_3} \cos 2\pi (z_w - z_{w+n}) \tag{5}$$

$$B_o = 0 \tag{6}$$

$$B_n = 2 \sum_{w=0}^{N_3} \sin 2\pi (z_w - z_{w+n}) \, , \tag{7}$$

where N_3 is the number of unit cells in the crystal in the c direction, N is the number of unit cells contained in a single reflecting plane, and the summation is taken over any column of unit cells defined by u and v equal to constants.

The deviation of the centroid position of the interference function from the reciprocal lattice point is given by

$$\bar{\zeta} = \frac{\int_{-\frac{1}{2}}^{\frac{1}{2}} \sum_{n=0}^{\infty} (A_n \cos 2\pi n\zeta + B_n \sin 2\pi n\zeta)\zeta d\zeta}{\int_{-\frac{1}{2}}^{\frac{1}{2}} \sum_{n=0}^{\infty} (A_n \cos 2\pi n\zeta + B_n \sin 2\pi n\zeta) d\zeta} \, . \tag{8}$$

Evaluation of equation (8) results in

$$\bar{\zeta} = \sum_{n=1}^{\infty} [(-1)^n / 2\pi n] B_n \, . \tag{9}$$

From equation (9) it would appear that $\bar{\zeta}$ is zero only for certain types of imperfect lattices, the most obvious being a lattice where positive and negative strains of the same magnitude are equally probable. Because, even for strains sufficiently small to have a good probability of existing in a cold worked metal, the elastic modulii depend on strain amplitude; the exact satisfaction of this type of strain distribution is not obvious. However, under certain quite general conditions it will be shown that the series of equation (9) converges to negligibly small values.

From equation (7) it follows that

$$B_1 = 2N_3 \{ -[(2\pi)^3/3!] \overline{\Delta z_1^3} + [(2\pi)^5/5!] \overline{\Delta z_1^5} - \dots \} \, , \tag{10}$$

where

$$\overline{\Delta z_1^3} = (1/N_3) \sum_{n=0}^{N_3} (z_n - z_{1+n})^3 .$$

From equation (3) it follows that

$$B_1 = (2/N) \int_{-\frac{1}{2}}^{\frac{1}{2}} I_0(\zeta) [2\pi\zeta - (2\pi\zeta)^3/3! + (2\pi\zeta)^5/5! - \dots] d\zeta \, . \tag{11}$$

Combining equations (10) and (11) we find

$$2\pi\bar{\zeta} = [(2\pi)^3/3!] [\overline{\zeta^3} - \overline{\Delta z_1^3}] - [(2\pi)^5/5!] [\overline{\zeta^5} - \overline{\Delta z_1^5}] + \dots . \tag{12}$$

If the interference function decreases to zero sufficiently rapidly as ζ increases, the third and all higher moments of the distribution are very small. Similarly, if the lattice strains between neighboring unit cells are sufficiently small, the higher moments of the strain distribution are negligible. Under these conditions $\bar{\zeta}$ is very nearly zero.

If we make the reasonable assumption that $\overline{\zeta^3}$ and $\overline{\Delta z_1^3}$ are both of the same order; an estimate of $\bar{\zeta}$ can be obtained for typical cold worked metals. For example, if we take $2 \cdot 10^{-3}$ as an upper limit for both $(\overline{\zeta^3})^{\frac{1}{3}}$ and $(\overline{\Delta z_1^3})^{\frac{1}{3}}$, then $\bar{\zeta} < 10^{-7}$, certainly a value which can be neglected.* Thus the percentage error introduced by approximating the reciprocal mean interplanar spacing by the position of the interference function centroid is about of the same order as the mean cubed strain between neighboring unit cells.

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* These values seem conservative, since by use of the Warren & Averbach analysis $(\overline{\Delta z_1^2})^{\frac{1}{2}}$, it is found to be of the order 10^{-2} to 10^{-3} for cold worked metals (Hirsch, 1956). The third moment should be much lower, of course, since positive and negative strains would partially cancel.

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A note on the heavy-atom method.

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In a recent paper (Sim, 1959) on the application of the heavy-atom method to non-centrosymmetric structures it was shown that improved resolution of the atoms could be obtained by employing in the Fourier series calculated from the phase angles α_H, amplitudes $W|F|$ rather than $|F|$, the weight W assigned to any term depending on the probable magnitude of the phase-angle error $(\alpha - \alpha_H)$. As the electron-density distribution is fairly insensitive to the precise set of weights adopted, any weighting function which increases smoothly from 0 to 1 as

$\langle|\alpha-\alpha_H|\rangle$ decreases from $\pi/2$ to 0 is probably satisfactory, and no attempt was made at the time to devise the best weighting function on the basis of a rigorous mathematical treatment, such as carried out by Woolfson (1956) for the centrosymmetrical case.

The weights which should be assigned to the structure amplitudes so that the mean-square error in electron density due to the phase-angle errors $(\alpha-\alpha_H)$ is minimized constitute what may be regarded as the best set of weights, and as the use of these weights puts the procedure on a more satisfactory theoretical basis they are derived here.

Following Blow & Crick (1959) it can be shown that these weights are defined by

$$W=\int_{-\pi}^{\pi}\cos\xi p(\xi)d\xi\ ,$$

where

$$\xi=\alpha-\alpha_H\ .$$

It was shown in the earlier paper that

$$p(\xi)=\exp\ (X\cos\xi)/2\pi I_0(X)\ ,$$

where

$$X=2|F|\,|F_H|/\Sigma_L$$

and consequently

$$W=I_1(X)/I_0(X)\ ,$$

where I_0 and I_1 are respectively the zero-order and first-order modified Bessel functions of the first kind (Watson, 1922, p. 77). Values of the weighting factor W are listed in Table 1. They differ from the earlier set in being consistently smaller for all values of X. Up to about $X=1{\cdot}5$ they agree fairly closely with the weights applicable to the centrosymmetrical case.

Table 1. *Values of the weighting factor W as a function of $X=2|F|\,|F_H|/\Sigma_L$*

X	0	0·25	0·50	0·75	1·0	1·5	2·0	3·0	4·0	5·0	∞
W	0	0·124	0·243	0·351	0·446	0·596	0·698	0·810	0·864	0·894	1·000

The use of the weighting procedure permits the inclusion from the beginning of a structure analysis of all the $|F_o|$ data. Moreover the calculation of the phase angles and of the electron-density distribution can be carried out consecutively without a break to select the data which are judged, in some more or less subjective manner, safe to be included in the Fourier calculation, an advantage when an electronic digital computing machine is available.

An example of the successful application of the method is provided by the analysis of the crystal structure of epi-limonol iodoacetate, $(C_{26}H_{31}O_8)COCH_2I$ (Arnott, Davie, Robertson, Sim & Watson, 1960), where, out of the 74 light atoms (neglecting hydrogen) in the asymmetric crystal unit, 50 were placed in the initial three-dimensional Fourier series calculated from phase angles based on the iodine atoms alone.

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Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the General Secretary of the International Union of Crystallography (Dr D. W. Smits, Laboratory of Inorganic and Physical Chemistry, 10 Bloemsingel, Groningen, The Netherlands).

The 18th Annual Meeting of the Electron Microscope Society of America

will be held August 29–31, 1960 in the Brooks Memorial Union Building at Marquette University, Milwaukee, Wisconsin.

In addition to the general sessions of contributed papers, it is planed to hold a special session of short papers on interesting, useful, and unusual electron microscopic techniques. Abstracts (limit—150 words) of papers for presentation at these sessions may be submitted to Professor W. C. Bigelow, EMSA Program Chairman, Department of Chemical and Metallurgical Engineering, University of Michigan, Ann Arbor, Michigan before May 15, 1960.

As special features of the meeting, three symposia are also being planned on: (1) 'The Structure of Teeth and Bone'—F. J. Sjöstrand, Chairman, (2) 'Recent Developments in Electron Metallography'—D. M. Teague, Chairman, and (3) 'Theory and Applications of Electron Diffraction'—G. R. Grieger, Chairman. These will include invited talks by experts on various topics in the fields covered by the symposia. There will also be extensive scientific and commercial exhibits.

Further information concerning the program of the meeting may be obtained from the Program Chairman. Information concerning the Scientific and Commercial Exhibits may be obtained from Dr Stanley Weinreb, EMSA Local Arrangements Chairman, Department of Anatomy, Marquette University School of Medicine, 516 North 15th Street, Milwaukee 3, Wisconsin.