which have to be carried out for each value of x. The necessary ranges of x and y must be considered and also the interval in these coordinates at which the summation is to be done. In the earlier papers the rule suggested for the choice of interval was that if H and K are sufficiently small they should be multiplied by factors to bring the product as near as possible to 20. This factor can then be regarded as multiplying θ, the interval of subdivision, and brings the latter up to a suitable value. The range of the strips is, of course, correspondingly increased. If H or K is less than 20 the strips need only to be added on the even sides, but if the maximum index H or K is greater than 20 then both even and odd sides should be added. In all such summations care must be taken to allow for the case where the number of $A(hk)$'s or $B(hk)$'s is reduced when $h = 0$ or $k = 0$ (see the Introduction to Lonsdale, 1936).

The 3° strips are also of considerable value in the calculation of structure factors, especially in the earlier stages of an analysis. In these stages it is convenient to keep the atoms to within 60ths or 120ths, when the strips can be used directly to give the values of the sums of terms like $\genfrac{}{}{0pt}{}{\cos}{\sin} 2\pi hx \,.\, \genfrac{}{}{0pt}{}{\cos}{\sin} 2\pi ky$. A strip can be selected to give first of all the values of $\cos 2\pi hx$ or $\sin 2\pi hx$, and these values can be used as the amplitudes of a $\cos 2\pi ky$ or $\sin 2\pi ky$ strip, which will give the answer for successive values of k. The strips for the various atoms can be laid beneath each other for convenience in adding. The accuracy obtainable by thus 'forcing' the atoms on to the nearest 6° or 3° is limited, and more accurate procedures are discussed by Sayre (1951) and by Beevers & Lipson (1952).

The calculation of molecular transforms also has its value in crystal-structure work, and this application of the strips has been described by Whittaker (1948).

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The Use of Fourier Strips for Calculating Structure Factors

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A method is described for using Fourier strips directly for the calculation of structure factors. The accuracy of the method is discussed, and some examples are given of the procedure involved.

1. Introduction

Much more attention seems to have been paid to the systematic calculation of electron densities in crystals than to the calculation of structure factors; the former operation is more easily dealt with, since it is concerned with precisely located points in the unit cell, whereas structure factors depend upon arbitrary positions. Nevertheless, when methods of evaluating electron densities had been satisfactorily worked out, the similarity of the electron-density equation

$$\varrho(x, y, z) = \frac{1}{V}\sum_h \sum_k \sum_l F(hkl) \exp\,[-2\pi i(hx+ky+lz)]$$

and the structure-factor equation

$$F(hkl) = \sum_n f_n \exp\,[2\pi i(hx_n+ky_n+lz_n)]$$

suggested to several workers (e.g. Robertson, 1936; Sayre, 1951) that these methods could be used for both operations.

There are, however, some difficulties associated with both these methods: Robertson's requires the preparation of 'sorting boards' for different atomic parameters, and Sayre's requires the careful preparation of an electron-density map representing the assumed structure. The present paper describes a more straightforward method, which can be put into operation by anyone who possesses a set of 3° Fourier strips.

2. General principles

In a sense, the method can be regarded as similar to that of Sayre (1951), who makes use of the fact that the weighted reciprocal lattice is the Fourier transform of the electron density in the crystal. This method can be used directly if we are prepared to place all the atoms on points whose coordinates are exact $\frac{1}{120}$ths of the unit cell, that is, with errors of the order of $\frac{1}{240}$ of the unit-cell edge. This is unsatisfactory for large unit cells, of the order of, say, 24 Å, since the errors in placing the atoms would be about 0·1 Å, although this would certainly be accurate enough for the initial stages of a structure determination; but for cell edges of the order of 6 Å the error in the positions of the atoms would be of the order of 0·02 Å, which is almost negligible. The present proposal, therefore, is to confine the use of the strips to the shorter axis only, so that only the smaller errors are introduced.

The principle can be best explained in terms of the structure-factor equation

$$F(hk0) = \sum_n f_n \cos 2\pi h x_n \cos 2\pi k y_n ,$$

which arises in many space groups. If all the atoms are similar, this may be written as

$$F(hk0) = f_n \sum_n \cos 2\pi h x_n \cos 2\pi k y_n .$$

Suppose that the unit cell has a long b cell dimension. Then the quantities $\cos 2\pi k y_n$ may be evaluated from tables, with any accuracy desired, for each atom and for each value of k. These quantities may then be used as amplitudes in the appropriate Fourier strips, the summation being effected in the usual way by placing the strips under each other and adding; successive columns give a row of structure factors with constant k and increasing h. The following are the rules of operation:

1. The amplitude of the strip is $\cos 2\pi k y$.
2. The index is the coordinate of the atom as an exact number of $\frac{1}{120}$ths.
3. Each column of the strip gives the contribution of the atom to successive structure factors.

The values of $\sum_n \cos 2\pi h x_n \cos 2\pi k y_n$ may then be multiplied by the appropriate values of scattering factor to give the structure factors required. Even if the atoms are not all similar, the derivation of the quantities $\cos 2\pi h x \cos 2\pi k y$ in this way is extremely helpful.

3. Improvement of the accuracy

For some purposes the accuracy of the method is insufficient, for the error in $\cos 2\pi h x$ due to an error δx is equal to $-2\pi h \delta x \sin 2\pi h x$, and so will tend to increase as h increases. The maximum error is $2\pi h \delta x$, and since δx may be as great as $\frac{1}{240}$, this maximum error is of the order of $h/40$, so that errors up to 20% will occur for indices of 8.

This accuracy may be considerably improved by a simple expedient, at the expense of doubling the computational work: if a parameter lies between two exact $\frac{1}{120}$ths, the weighted mean of these two is taken. Thus if the parameter is $p/120$, where p is not integral, it is expressed as

$$p = \frac{n_1(p+n_2)+n_2(p-n_1)}{n_1+n_2} ,$$

where $p+n_2$ and $p-n_1$ are integral and $n_1+n_2 = 1$. Thus instead of one strip, two adjacent strips, of amplitude $\{n_1/(n_1+n_2)\} \cos 2\pi k y$ and $\{n_2/(n_1+n_2)\} \cos 2\pi k y$, and of indices $p+n_2$ and $p-n_1$ respectively, are chosen.

The error is obviously a maximum if $n_1 = n_2$, when it can be shown that the accuracy depends upon the degree to which $\cos \{2\pi h n_1/120\} = 1$. Thus up to $h = 6$ the maximum error is only 1% and up to $h = 12$ it is only 5%. If errors of this amount (which is probably equal to that with which the scattering factors of the various atoms are known) can be tolerated, then it may be worth while using the strips so that they correspond to the *larger* range of index; if they correspond to the smaller range, only a few columns of the strips are used and the extraction and replacement of the strips may take more time than the additions.

4. Modification for parameters greater than 0·25

The 3° strips prepared by Beevers (1952) include indices only up to 30, which corresponds to a parameter of 0·25. If a parameter lies between 0·25 and 0·50, however, the strips can be used quite simply; in place of index p, the index $60-p$ is chosen; the even places on the strip (on the obverse side) then give the values required, and for cosine summations the odd places (on the reverse side) give the negatives of the values required. Parameters lying between 0·50 and 1·00 may be expressed as negative quantities

Table 1. *Extension of the strips to cover the whole unit cell*

		p	$60-p$	$p-60$	$120-p$
Cos	Even places	+	+	+	+
	Odd places	+	−	−	+
Sin	Even places	+	−	+	−
	Odd places	+	+	−	−

Table 3. *Example of structure-factor calculation*

	020	220	420	620	820	...
83 CE 15	83	0	$\overline{83}$	0	83	...
62 CE 17	62	$\overline{13}$	$\overline{57}$	36	41	...
$\overline{62}$ CE 4	$\overline{62}$	57	$\overline{41}$	$\overline{19}$	6	...
	83	$\overline{70}$	$\overline{181}$	17	130	...
$\overline{92}$ CE 13	$\overline{92}$	$\overline{19}$	84	54	$\overline{62}$	...
Sum	$\overline{9}$	$\overline{89}$	$\overline{97}$	71	68	...

	120	320	520	720	920	...
83 CO 15	59	$\overline{59}$	$\overline{59}$	59	59	...
62 CO 17	39	$\overline{55}$	$\overline{16}$	62	$\overline{10}$	...
$\overline{62}$ CO 4	$\overline{61}$	$\overline{50}$	$\overline{31}$	$\overline{6}$	19	...
	37	$\overline{164}$	$\overline{106}$	115	68	...
$\overline{92}$ CO 13	$\overline{71}$	42	89	$\overline{5}$	$\overline{91}$	...
Difference	108	$\overline{206}$	$\overline{195}$	120	159	...

Table 4. *Example of improved accuracy*

	020	220	420	620	820	
63 CE 15	63	0	$\overline{63}$	0	63	...
20 CE 14	20	2	$\overline{20}$	$\overline{6}$	18	...
59 CE 17	59	$\overline{12}$	$\overline{54}$	35	39	...
3 CE 18	3	$\overline{1}$	$\overline{2}$	2	1	...
$\overline{37}$ CE 4	$\overline{37}$	$\overline{34}$	$\overline{25}$	$\overline{11}$	4	...
$\overline{25}$ CE 3	$\overline{25}$	$\overline{24}$	$\overline{20}$	$\overline{15}$	$\overline{8}$	...
	83	$\overline{69}$	$\overline{184}$	5	117	
$\overline{52}$ CE 13	$\overline{52}$	$\overline{11}$	48	31	$\overline{35}$	
$\overline{41}$ CE 14	$\overline{41}$	$\overline{4}$	40	13	$\overline{37}$	
	$\overline{93}$	$\overline{15}$	88	44	$\overline{72}$	
Sum	$\overline{10}$	$\overline{84}$	$\overline{96}$	49	45	

	120	320	520	720	920	
63 CO 15	45	$\overline{45}$	$\overline{45}$	45	45	...
20 CO 14	15	$\overline{12}$	$\overline{17}$	8	19	...
59 CO 17	37	$\overline{53}$	$\overline{15}$	59	$\overline{9}$	...
3 CO 18	2	$\overline{3}$	0	3	$\overline{2}$	...
$\overline{37}$ CO 4	$\overline{36}$	$\overline{30}$	$\overline{18}$	4	11	...
$\overline{25}$ CO 3	$\overline{25}$	$\overline{22}$	$\overline{18}$	$\overline{11}$	$\overline{4}$	...
	38	$\overline{165}$	$\overline{113}$	100	60	
$\overline{52}$ CO 13	$\overline{40}$	24	50	$\overline{3}$	$\overline{51}$	
$\overline{41}$ CO 14	$\overline{30}$	24	36	$\overline{17}$	$\overline{39}$	
	$\overline{70}$	48	86	$\overline{20}$	$\overline{90}$	
Difference	108	$\overline{213}$	$\overline{199}$	120	150	

and so brought also within the range of the procedure. For sine summations the changes of sign are different, and the various cases are given in Table 1.

The function $\cos 2\pi(hx+ky)$ is most conveniently dealt with by expansion into the form $\cos 2\pi hx \cos 2\pi ky - \sin 2\pi hx \sin 2\pi ky$. This does not double the work, because the structure factors $hk0$ and $h\bar{k}0$ can be derived from the same calculations.

5. Examples

A simple example is given to show the method of calculation. Consider a crystal with plane group *pmm* having atoms with the parameters shown in Table 2.

Table 2. *Assumed parameters in decimals and in* $\frac{1}{120}$*ths*

	Decimals	$\frac{1}{120}$ths	$\cos 2\pi ky$
x_1	0·123	14·76	—
y_1	0·047	—	0·831
x_2	0·142	17·04	—
y_2	0·428	—	0·618
x_3	0·030	3·60	—
y_3	0·322	—	−0·618
x_4	0·388	46·56	—
y_4	0·220	—	−0·925

Lists of the values of $\cos 2\pi ky$ may be made; the values for $k = 2$ are given in Table 2.

The summations for the $h20$ reflexions up to $h = 9$ are shown in Table 3.

The weighting procedure can be demonstrated by the same example (Table 4).

The accuracy of the two procedures is shown by the comparison of the two sets of results with the values obtained by ordinary calculation to three decimal places (Table 5).

It will be seen that, while the first method gives results which are useful for preliminary work only, the second gives results that are, over the range of calculation, of quite adequate accuracy. Since the methods reduce the calculations to the simple selection and addition of strips, they should speed the work of calculation considerably.

Table 5. *Comparison of values of* $\Sigma \cos 2\pi hx \cos 2\pi ky$ *obtained by three different methods*

hkl	First method	Second method	Accurate calculation
020	−0·09	−0·10	−0·09
120	1·08	1·08	1·08
220	−0·89	−0·84	−0·84
320	−2·06	−2·13	−2·11
420	−0·97	−0·96	−0·97
520	1·95	−1·99	−2·00
620	0·71	0·49	0·48
720	1·20	1·20	1·19
820	0·68	0·45	0·46
920	1·59	1·50	1·53

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