for 222. By using the temperature factor $B=0{\cdot}46$ Å^2 (at 293°K) obtained by Aldread & Hart (1973), the crystal structure factors including the sign are calculated to be $F_{111}=59{\cdot}87\pm0{\cdot}46$ and $F_{222}=-1{\cdot}85\pm0{\cdot}85$ at 293°K. The present value of F_{111} is smaller by about 1% compared to the most accurate data from X-rays (Tanemura & Kato, 1972; Aldread & Hart, 1973), whereas that of F_{222}, which is due to the antisymmetric part of the charge distribution (Dawson, 1967), is larger than all the available data as seen in Table 3.

Table 3. *The structure factors F_{111} and F_{222} at room temperature converted from the original data*

Source	Method	F_{111}	F_{222}
G. & W. (1959)	X-ray Int.	$60{\cdot}81\pm0{\cdot}11$	$1{\cdot}12\pm$? *
D. & W. (1965)	X-ray Int.	$60{\cdot}47\pm0{\cdot}45$	$1{\cdot}44\pm0{\cdot}08$*
H.K.K.K. (1965)	X-ray Dyn.	$62{\cdot}12\pm0{\cdot}93$	$-1{\cdot}44\pm0{\cdot}08$†
T. & K. (1972)	X-ray Dyn.	$60{\cdot}32\pm0{\cdot}01$	
A. & H. (1973)	X-ray Dyn.	$60{\cdot}32\pm0{\cdot}03$	$-1{\cdot}35\pm0{\cdot}04$†
Cowley (1969)	Electr. Dyn.	$60{\cdot}36\pm$?	$-0{\cdot}07\pm$?
K. & M. (1971)	Electr. Dyn.	$59{\cdot}97\pm0{\cdot}05$	$-1{\cdot}6\ \pm0{\cdot}2$
Present (1974)	Electr. Dyn.	$59{\cdot}87\pm0{\cdot}46$	$-1{\cdot}85\pm0{\cdot}85$

* The sign has not been determined.
† Theoretical values calculated by Dawson's (1967) formula.

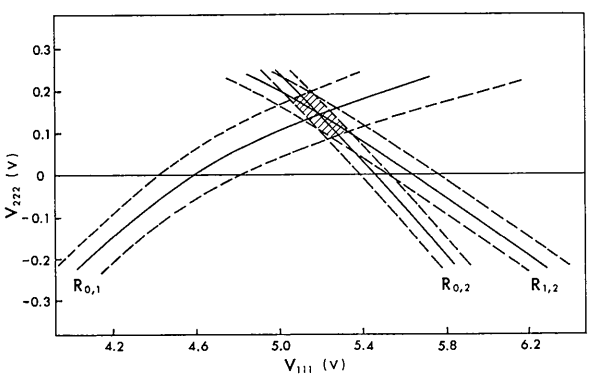

Fig. 1. Determination of V_{111} and V_{222} of silicon at 392 kV. The ratios of the fringe distances $R_{0,1}$, $R_{0,2}$ and $R_{1,2}$ are listed in Table 1. A pair of broken lines are drawn corresponding to the errors of each ratio.

In the above analysis, it was shown that the sign of the structure factor for centrosymmetric crystals can be determined by electron-dynamical methods by taking account of many-beam effects. Cowley's (1969) method is similar to the present one, but it does not seem adequate for accurate determination. Although Kreutle & Meyer-Ehmsen's (1971) method gives high accuracy, a highly refined technique of intensity measurement is required. On the other hand, the present method needs only the measurement of the fringe spacings in the electron micrographs. By a similar method, one of the present authors has recently determined the phase angle of the structure factor for the 0002 reflexion in cadmium sulphide, which has no centre of symmetry. Details of the experiments for silicon and cadmium sulphide will be published elsewhere in the near future.

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Treatment of negative indices in crystallographic fast Fourier transforms.

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An algorithm for fast Fourier transformation using sequentially organized backing storage is described; a simple modification has been made to an existing procedure, to allow the Fourier coefficients to have negative indices, without the need to introduce additional phase factors. A general purpose crystallographic FFT program has been written for a 16K IBM 1130 with three disks.

There has been some interest in applying the fast Fourier transform (FFT) to crystallography since its discovery by Cooley & Tukey (1965). Methods have been described for incorporating the space-group symmetry (Ten Eyck, 1973), and for using backing store to accommodate the array of data (Singleton, 1967; Lange, Stolle & Huttner, 1973). The general formula is

$$\varrho(x,y,z)=\sum_{h=h_a}^{h_e}\sum_{k=k_a}^{k_e}\sum_{l=l_a}^{l_e}F_{hkl}\exp-2\pi i\varphi$$

where

$$\varphi=hx/N+ky/O+lzP \qquad (1)$$

$$N=h_e-h_a;\quad O=k_e-k_a;\quad P=l_e-l_a;$$

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h,k,l are the indices of the Fourier coefficient F_{hkl}; (h_a,h_e), (k_a,k_e), (l_a,l_e) are the limits of the indices; $\varrho(x,y,z)$ is the value of the transform at discrete coordinates x, y, and z. To use the FFT for such computations two steps are necessary: (i) split up the multiple sum into single sums, and (ii) convert the negative indices into positive indices.

Singleton (1967) performs multidimensional transforms of the form of equation (1), in which $h_a=k_a=l_a=0$ and $h_e=2^a$; $k_e=2^b$; $l_e=2^c$. He regards the three-dimensional array of Fourier coefficients as a single one-dimensional array with F_{hkl} stored at location,

$$\text{Loc}\,(F_{hkl})=h+(k+2^b l)2^a\,. \tag{2}$$

The computation is done in $n=a+b+c$ computing passes of the array. On the kth pass data points 2^{n-k} apart are transformed and the results stored in an output array in locations 2^{n-1} apart. The transform is

$$\begin{aligned} Y_j &= x_j + x_{j'}\,\exp\,[-i\pi(j\div 2^{n-k'})/2^{k'-1}] \\ Y_{j+2^{n-1}} &= x_j - x_{j'}\,\exp\,[-i\pi(j\div 2^{n-k'})/2^{k'-1}]\,, \end{aligned} \tag{3}$$

where $j'=j+2^{n-k}$

$$\begin{aligned} k' &= k \quad \text{if} \quad 0<k\le a \\ &\quad k-a \quad \text{if} \quad a<k\le a+b \\ &\quad k-a-b \quad \text{if} \quad a+b<k\le a+b+c \end{aligned}$$

and $\div$ denotes integer division. The x_j are the values of the input array and the y_j are the values to be stored in the output array. This output array is held in sequential backing store on two files used as input for the next pass. After n passes $\varrho(x,y,z)$ is stored at location

$$\text{Loc}\,[\varrho(x,y,z)]=z+(y+2^b x)2^c\,. \tag{4}$$

Lange, Stolle & Huttner (1973) deal with the crystallographic case where h_a, k_a and l_a may be negative. They modify each row of the array of coefficients by an additional phase factor depending on the row index. This requires an extra computing pass of the data, with the evaluation of an exponential factor for each row. We suggest here a more economical technique, utilizing the periodic property of the Fourier transform.

The region of reciprocal space bounded by the experimental sphere circumscribes a parallelepiped with sides of length Na^*, Ob^* and Pc^* r.l.u., where a^*,b^*,c^* are the reciprocal-lattice translations. Since this diffraction space is finite and discrete (the reciprocal transform has zero amplitude except at the discrete reciprocal-lattice points), its Fourier transform ϱ is periodic with periods N,O,P along the x, y and z axes respectively. The Fourier coefficient F_{hkl} is defined only for

$$h_a\le h\le h_e,\ k_a\le k\le k_e,\ l_a\le l\le l_e$$

but can be defined for all indices by

$$F_{h'k'l'}=F_{hkl} \tag{5}$$

where

$$h'=n_1N+h;\ k'=n_2O+k;\ l'=n_3P+l$$

and

$$n_1,n_2,n_3=0,\pm 1,\pm 2,\ldots\,.$$

It is now periodic with the same period as ϱ and the transform of any complete period is ϱ. To compute the transform consider the period

$$0\le h<N,\ 0\le k\le O,\ 0\le l<P\,.$$

This is obtained by adding N (respectively O,P) to negative h (respectively k,l) indices. Thus to adapt Singleton's multidimensional method to cope with negative indices it is only necessary to alter the address function (2) to

$$\text{Loc}\,(F_{hkl})=h'+(k'+l'O)N \tag{6}$$

where

$$\begin{aligned} h' &= h \quad \text{if} \quad h\ge 0 \\ &\quad h+N \quad \text{if} \quad h<0 \\ k' &= k \quad \text{if} \quad k\ge 0 \\ &\quad k+O \quad \text{if} \quad k<0 \\ l' &= l \quad \text{if} \quad l\ge 0 \\ &\quad l+P \quad \text{if} \quad l<0\,. \end{aligned}$$

After n computing passes using the same transform (3) the complete period

$$0\le x<N,\ 0\le y<O,\ 0\le z<P$$

of the Fourier transform is stored in the output array with the address function (4).

The above algorithm is the basis of a general crystallographic FFT program written in Fortran for an IBM 1130 computer with 16K core store and three disk drives. Transform time for 2^{15} data points is 70 min; this could be reduced by the use of a fourth disk drive.

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