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A new graphical principle for the evaluation of Fourier transforms.

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It has been shown (Grenville-Wells, 1954) that if in a [001] projection of a unit cell the normal to the planes $(hk0)$ is graduated with a sine or cosine function whose period is that of the interplanar spacing, then a circle with its centre at $(\frac{1}{2}x, \frac{1}{2}y)$, passing through the origin, will cut the normal to $(hk0)$ at the value of $\sin 2\pi(hx+ky)$ or $\cos 2\pi(hx+ky)$, and that this offers a very rapid graphical method of evaluating structure factors like $F(hk0)$.

This note describes the application of the same geometrical principle to the calculation of structure factors at non-integral as well as integral values of h and k, thus permitting the rapid evaluation of Fourier transforms.

In a square [001] projection of the unit cell of a crystal (Fig. 1(*a*)) the traces of the planes $(hk0)$, where k is constant ($k = 2$ in Fig. 1(*a*)), will radiate from the point A. The normals $F(0, 2)$, $F(1, 2)$ and $F(2, 2)$ to these planes intersect the planes themselves at points A, B and C which lie on the circle $OABC$ having its centre at P and of radius $OP = \frac{1}{2}OA$. It follows that if k is kept constant, the circle $OABC$ is the locus of the first maximum, along the normal to $(hk0)$, of the function $\cos 2\pi(hx+ky)$ for all values of h, whether integral or non-integral.

Thus if the line $F(0, k)$ is graduated as finely as desired (at 15° intervals in the chart shown in Grenville-Wells (1954)), and each graduation is made the diameter of a circle, a chart of the type shown in Fig. 1(*b*) will result, i.e. a chart for evaluating the set of structure factors $F(hk0)$ having a common index k for all values of h from 0 to k. On it any selected $F(hk)$ line (like OQ = $(F0{\cdot}6, 2{\cdot}0)$ in the diagram) is thereby graduated, $F(h, k)$ being the line through O making an angle $\tan^{-1}(h/k)$ with OY. This graduated line is then used to find the value of the corresponding structure factor, as described in the paper quoted above.

A single chart of this type can be used to evaluate structure factors accurately up to very high orders, since the value of the function $\cos 2\pi(hx+ky)$ is obtained either from the intersection of the line $F(h, k)$, divided into $(h+k)$ parts, with the circle centred at $(\frac{1}{2}x, \frac{1}{2}y)$; or from the intersection of a line of the same length divided into $(h+k)/n$ parts and the circle centred at $(\frac{1}{2}nx, \frac{1}{2}ny)$. For example, in Fig. 1(*b*) the line OQ could be used to obtain $F(3, 10)$ with a set of circles centred at $(5x/2, 5y/2)$.

As would be expected, much greater accuracy is obtained by drawing several sets of circles for successive multiples of the atomic co-ordinates in a trial structure (which only takes a few minutes per set) and using them in conjunction with a few carefully drawn large-scale charts of this type, than by trying to graduate high-order $F(hk0)$ charts accurately.

Constant-k charts of this type thus have an advantage over charts on which $F(hk0)$ lines are drawn for different values of both h and k, in that they can be used both for structure factors (integral values of h and k) and Fourier transforms (non-integral values of h and k). As in Grenville-Wells (1954), interchange of the x and y axes, by reversing the tracing carrying the circles, converts the constant-k charts into constant-h charts.

References

Grenville-Wells, H. J. (1954). *J. Appl. Phys.* **25**, 485.

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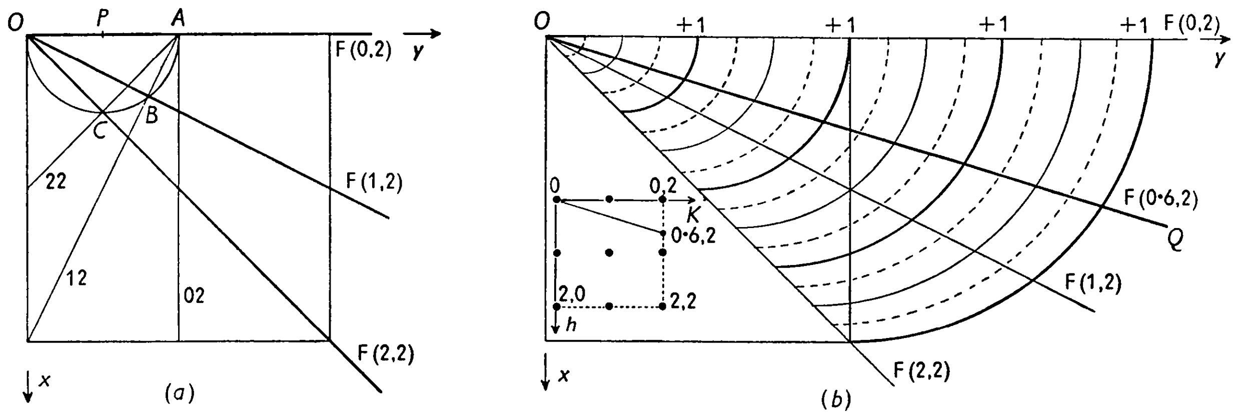

Fig. 1.