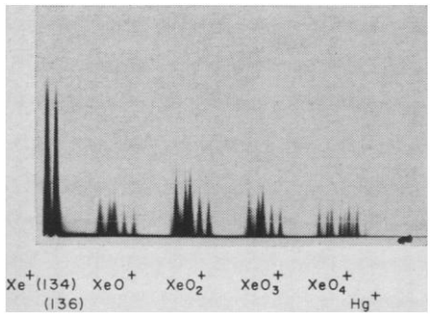

Fig. 1. Mass spectrum of xenon tetroxide.

spectrum of mercury. The fragmentation pattern varied very little with the energy of the ionizing beam of electrons.

The volatility of XeO_4 was demonstrated by its very rapid distillation when a liquid nitrogen bath was replaced by one of dry ice.

The same reaction conducted in a test tube yields a gas with a strong pungent odor which gives a test with potassium iodide-starch paper. These properties could be caused by ozone; however, only a small peak was observed at mass 48 in the mass spectrometer.

JOHN L. HUSTON
Loyola University, Chicago, Illinois
MARTIN H. STUDIER
ERIC N. SLOTH
Chemistry Division, Argonne National Laboratory, Argonne, Illinois 60440

References and Notes

1. J. G. Malm, R. W. Bane, B. D. Holt, in *Conference on Noble Gas Compounds, Proceedings*, H. H. Hyman, Ed. (Univ. of Chicago Press, Chicago, 1963), pp. 167–173.
2. M. H. Studier and E. N. Sloth, *ibid.*, pp. 47–49; M. Studier, *Rev. Sci. Instr.* **34**, No. 12, 1367 (1963).
3. Based on work performed under the auspices of the U.S. Atomic Energy Commission. We thank J. G. Malm for the sample of sodium perxenate and L. P. Moore for technical assistance.

30 December 1963

Computer Program for Printing Undeformed Fourier Maps

Abstract. *The program calculates the values of the function at those points where the computer can print them.*

A doubly periodic function that can be represented by a Fourier series with known coefficients is usually computed at m by n points in the mesh (two-dimensional period). The mesh, a parallelogram in the general case, has each of its sides subdivided into an integral number of parts, m or n. The machine prints the results in a rectangular array, which is a deformed map of the mesh. The deformation has two sources: (i) the map cannot be true to scale in both directions and (ii) the parallelogram is transformed into a rectangle.

The purpose of the program is to print an array of numbers that can be contoured directly into a map, on which true distances and angles can be measured. Two cases can be considered. In one the mesh is orthogonal (a rectangle) and in the other it is nonorthogonal (a parallelogram).

Orthogonal mesh. For example, *ca* in the orthorhombic system, with $c < a$.

The problem is one of scale only. In general, for any convenient scale, say 1 Å to 2 inches, c will be a nonintegral multiple M of the width of one machine-printed digit (or interval), and a will be another nonintegral multiple N of some interline spacing (single, double, . . .). The machine will be asked to calculate the values of the doubly periodic function precisely at the points where they can be printed. These points form a rectangular array, which we will call the "machine grid." Successive rows come at $x = pa/M$, where

$$p = 0, 1, 2, \ldots, m, m+1$$

and $m < M < m + 1$. Along each row, points come at $z = rc/N$, where

$$r = 0, 1, 2, \ldots, n, n+1$$

and $n < N < n + 1$.

The summation of the Fourier series at the points of the machine grid can be shortened thanks to a recurrence formula of H. Takahashi (*1*). To calculate either

$$C = \tfrac{1}{2}\, a_0 + \sum_{h=1}^{H} a_h \cos 2\pi hX$$

or

$$S = \sum_{h=1}^{H} a_h \sin 2\pi hX$$

(note that the coefficients a_h need not be the same in S as in C), compute the following sequence of u_n's:

$$\begin{aligned}
u_0 &= \qquad\qquad\qquad\quad a_H,\\
u_1 &= 2\,u_0 \cos 2\pi X \qquad + a_{H-1},\\
u_2 &= 2\,u_1 \cos 2\pi X - u_0 \quad + a_{H-2},\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots,\\
u_n &= 2\,u_{n-1} \cos 2\pi X - u_{n-2} + a_{H-n},\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots,\\
u_{H-2} &= 2\,u_{H-3} \cos 2\pi X - u_{H-4} + a_2,\\
u_{H-1} &= 2\,u_{H-2} \cos 2\pi X - u_{H-3} + a_1,\\
u_H &= 2\,u_{H-1} \cos 2\pi X - u_{H-2} + a_0,
\end{aligned}$$

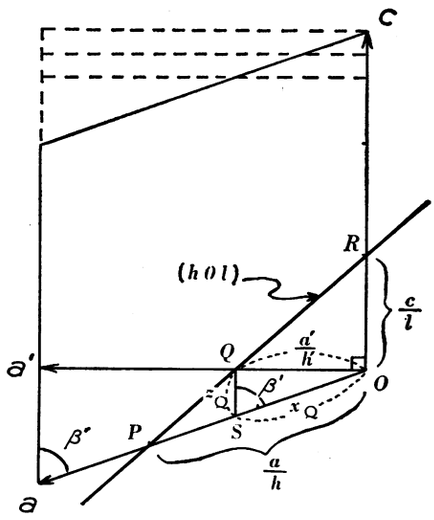

Fig. 1. Monoclinic mesh *ca*, with trace of (*h*0*l*) plane and intercepts of the latter on a, a', and c, equal to OP, OQ, and OR, respectively.

but keep only the last three values. Then C or S, as the case may be, is given by,

$$C = \tfrac{1}{2}\,(u_H - u_{H-2})$$

or by

$$S = u_{H-1} \sin 2\pi X.$$

Although the Takahashi formula was proposed for a small computer and for calculations that made use of an integral number of subdivisions in the period (for example, $M = m = 45, 60, 100, \ldots$; with $X = 1/M$), its main advantages are that it permits the use of a nonintegral number of subdivisions and that it eliminates the looking up of sine and cosine tables, which is usual in the Beevers-Lipson summation method.

Non-orthogonal mesh. For example, *ca* in the monoclinic system, with $a < c$.

The mesh is a parallelogram. In view of the fact that the translation repeat need not have the same shape as the mesh, we propose, for purposes of computation, that the repeat of the Fourier function be taken as a rectangle instead of a parallelogram. This result can be achieved by using nonintegral Miller indices (*h*0*l*). For example, the parallelogram *ca* can be replaced by the rectangle *ca'* (Fig. 1), where

$$a' = a \sin \beta'$$

and

$$a'/h' = x_Q \sin \beta',$$

with $\beta' = 180° - \beta$. Symbol $(h0l)$ transforms to $(h'0l)$. From the equation of the trace of the $(h0l)$ plane and the equation of $0a'$,

$$h(x/a) + l(z/c) = 1$$

and

$$z = x \cos \beta',$$

we find x_Q, the abscissa of the point of intersection Q of the two lines. We then obtain

$$h' = h + ql,$$
$$q = (a/c) \cos \beta'.$$

As an example let us take the calculation of a two-dimensional Fourier series in "ferri-annite," a one-layer monoclinic synthetic iron mica,

$$KFe_3^{2+} (Si_3Fe^{3+}) O_{10} (OH)_2,$$

which crystallizes in space group $C2/m$. With the axes zx' and the mesh ca', the electron-density projection onto (010) is given by (2):

$$\rho(x',z') = \frac{1}{A} \sum_{l'} \sum_{h'} F(h'0l') \times \cos 2\pi \left(h' \frac{x'}{a'} + l' \frac{z'}{c}\right),$$

(where $A = ca' = ca \sin \beta'$ is the mesh area) or, replacing h' by its value and noting that $F(h'0l') = F(h0l)$, by

$$\rho(x',z') = \frac{1}{A} \sum_{l} \sum_{h} F(h0l) \times \cos 2\pi \left[(h + ql) \frac{x'}{a'} + l \frac{z'}{c}\right],$$

where $(h0l)$ refers to the mesh ca.

For the practical summation we write

$$\rho(x',z') = \frac{2}{A} \left(\sum_{l=0}^{L} C'_l \cos 2\pi l \frac{z'}{c} \right) - \frac{2}{A} \left(\sum_{l=l}^{L} S'_l \sin 2\pi l \frac{z'}{c} \right),$$

with

$$C'_l = C_l \cos 2\pi ql \frac{x'}{a'} - S_l \sin 2\pi ql \frac{x'}{a'},$$

$$S'_l = S_l \cos 2\pi ql \frac{x'}{a'} + C_l \sin 2\pi ql \frac{x'}{a'},$$

and

$$C_l = F(00l) + \sum_{h=1}^{H} [F(h0l) + F(\bar{h}0l)] \times \cos 2\pi h \frac{x'}{a'},$$

for $l > 0$,

$$C_0 = \tfrac{1}{2} F(000) + \sum_{h=1}^{H} F(h00) \cos 2\pi h \frac{x'}{a'},$$

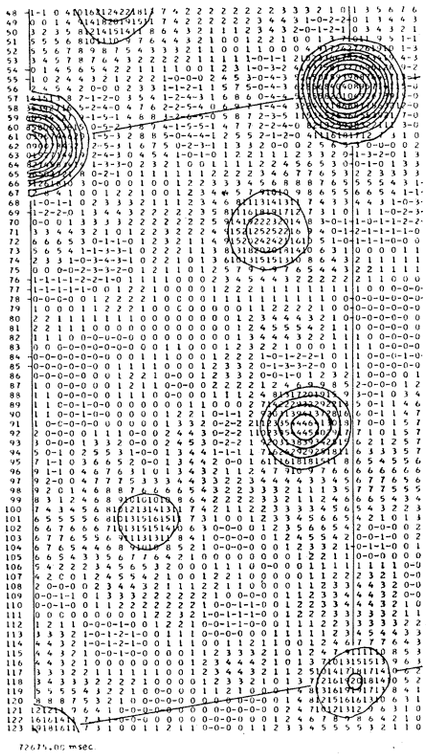

Fig. 2. Electron-density projection of monoclinic mica "ferri-annite" onto ca' plane. The parallelogram (or asymmetric domain) is one-quarter of the mesh. Contours are drawn directly on the print-out. x' increases from left to right, z' from top to bottom (see numbers along left edge).

for $l = 0$,

$$S_l = \sum_{h=1}^{H} [F(h0l) - F(\bar{h}0l)] \sin 2\pi h \frac{x'}{a'}.$$

The summations C_l and S_l are carried out over integral values of h; they are given the ordinary summation formulas for space group $C2/m$. The only change required by introduction of the nonintegral h' indices is that, in summations over l, the coefficients C'_l and S'_l must be used instead of C_l and S_l.

The value of q is constant for a given mesh ca, so that for fixed l and (x'/a'), the sine and cosine of $2\pi ql(x'/a')$ are also constant. In order to avoid having to compute these values for every l and (x'/a'), we use the formulas for the cosine and sine of the sum of two angles, in the following form:

$$\cos 2\pi \frac{p+1}{M} = \cos 2\pi \frac{p}{M} \cos 2\pi \frac{1}{M} - \sin 2\pi \frac{p}{M} \sin 2\pi \frac{1}{M},$$

$$\sin 2\pi \frac{p+1}{M} = \sin 2\pi \frac{p}{M} \cos 2\pi \frac{1}{M} + \cos 2\pi \frac{p}{M} \sin 2\pi \frac{1}{M},$$

where M is the number (not necessarily integral) of subdivisions in the period and p is an integer. These formulas have to be applied twice, as l and (x'/a') are made to increase. They are also used to compute $\cos 2\pi X$ and $\sin 2\pi X$, which are needed in Takahashi's formulas.

The next step is to produce an undeformed map. This is done as in the case of the orthogonal mesh (see above). The map obtained (Fig. 2) is on the scale of 1 angstrom to 2 inches on the print-out. The horizontal edge a' was divided into 53.475 parts; the vertical edge c, in 123.84 parts. With two digits the value of the function may increase from -9 to 109 (printed as 09).

For a three-dimensional triclinic synthesis, the method could be generalized, the triclinic cell being replaced by a rectangular parallelepiped, or else printed rectangular sections could be stacked with the appropriate offset for the inter-section spacing.

J. D. H. Donnay
Hiroshi Takeda
Crystallographic Laboratory,
Johns Hopkins University,
Baltimore 18, Maryland

References and Notes

1. Y. Iitaka and T. Sakurai, *Kobutsu-gaku Zasshi* **4**, 409 (1960).
2. Although the z axis remains the same ($c' = c$), the z coordinate changes and is therefore designated z'. Thus $z'/c \neq z/c$, but $x'/a' = x/a$.
3. Paper presented at a symposium of the International Union of Crystallography, Rome, Italy, 17 Sept. 1963. Work supported by the National Science Foundation (GP 1565). Computations performed on I.B.M. 7094 at the Johns Hopkins computation center. Gabrielle Donnay and Charles W. Burnham kindly read the manuscript.

29 October 1963

Natural Carbon-14 Activity of Organic Substances in Streams

Abstract. *Carbon-14 measurements made on organic contaminants extracted from streams show percentages of industrial waste and domestic sewage. The method, used previously for studies of the atmosphere, can be used in studies of pollution sources.*

The two most important sources of organic chemical pollution of water are industrial wastes and domestic effluents (sewage). It is desirable to distinguish between these substances in streams in order to plan abatement measures, for they injure water quality in different ways. By recovering the organic substances from a polluted stream