[110] and [1 $\overline{10}$], whilst [010], being the twofold axis of the space group, reproduces the crystal without twinning. The unique twin axes are therefore [100], [130] and [110].

All these have been observed experimentally, [110] by Barth & Balk (1934), [130] by Milne (1949) and Hietanen (1951), all in optical measurements, and [100] in the present work. In addition, Hietanen lists three further axes, [120], [210] and [310], the result of optical measurements on chloritoid from Rawlinsville, Lancaster Co., Pennsylvania, U.S.A., which, if correct, suggest the existence of at least one other structural form of chloritoid.

We are indebted to Dr F. A. Bannister of the British Museum for supplying the sample of chloritoid on which this investigation was made, to Dr H. L. Lovell of the College of Mineral Industries, The Pennsylvania State University, U.S.A., for recording the infra-red absorption spectrum, and to Dr W. H. Taylor of the Cavendish Laboratory, Cambridge, England, who made available computational facilities for the final (0kl) synthesis.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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An analogue computer for double Fourier series summation for X-ray crystal-structure analysis. By G. Suryan, Department of Physics, Indian Institute of Science, Bangalore 3, India

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The need for computational aids in the determination of crystal structures by means of X-ray diffraction studies has been keenly felt by all workers in the field and probably there are as many devices as there are workers, with varying degrees of accuracy, usefulness, complexity and cost. Of these the X-RAC machine built by Pepinsky (1952) has generally been acclaimed the best and would have found wide application but for its expense. It is the object of this note to show that a system which is relatively much less expensive than the X-RAC machine could be devised, based on the general principles of the synchronous magnetic recorder devised by the author (Suryan, 1950, 1953a, b), without any particular loss in performance.

The problem is to find the sum $\varrho(x,y)$ of a double Fourier series of given coefficients F_{hk} and phases α_{hk} of the form $\Sigma\Sigma F_{hk}$ cos/sin $2\pi(hx/a+\alpha_{hk})$ cos/sin $2\pi(ky/b)$

over the domain x = 0 to x = a and y = 0 to y = b at close enough intervals, and to present the results preferably in the form of a contour map of the function $\hat{\varrho}(x, y)$. Electrical sine waves are the most suitable analogues to the cos/sin functions, and the analogy can be effected by the transformation of the x, y domain into time by means of two transformations x/a = pt and y/b = $p't(p \gg p')$, corresponding to a fast and slow scan of the x, y domain respectively. Then one set of harmonically related electrical waves may represent the $\cos/\sin 2\pi (hx/a)$ and a set of cosine resolvers suitably ganged through a gearbox may perform the function of generating the second set $\cos/\sin 2\pi (ky/b)$. To utilize these analogues in their most primitive form one would require a large number of oscillators and much larger number of amplitude controls and a multitude of adding amplifiers etc., all going to make the equipment prohibitively expensive

and complex. It is here that the basic principles of the synchronous magnetic recorder could be utilized with advantage; a computer system has been designed on that basis and a programme of development and construction has been going on at the Physics Department, Indian Institute of Science, Bangalore, for more than two years. Fig. 1 gives a self-explanatory block schematic of the system. The new ideas employed therein have been individually tested and found to work satisfactorily. The following are the salient points of the system:

- (a) The basic data F_{hk} are recorded on a rotating magnetic drum in the form of sine waves (which are in synchronism with the rotation of the drum) of suitable phases and amplitudes. As the terms of the double Fourier series are recorded individually and in succession the necessity for a large number of oscillators and much larger number of amplitude controls ceases. One set of chopper discs is used to generate the sine waves photoelectrically.
- (b) Pure sine waves without distortion are recorded, as the waves are in synchronism with the rotation of the drum and suitable magnetic negative feed-back is applied to attain linearity of response. Briefly the method is as follows. The basic frequency (i.e. h=1) is chosen to be double the frequency of rotation of the drum. Then a pick-up situated at a point diametrically opposite to that of the recording head picks up the recorded signal, and that is compared with the input signal and suitable correcting signals are applied automatically.

- (c) The first summation of the double Fourier series is easily made by recording the individual terms of the sub-sum near one another and providing a common long pick-up head. The pick-up heads are made with low output impedance such that they (combined with the large peripheral velocity of the drum) give enough output to feed directly into the cosine resolvers (ganged through a gearbox), thus generating the second set of harmonically related sin/cos functions and multiplying them into the original sin/cos functions.
- (d) One final adding amplifier adds and amplifies the output of the cosine resolvers.
- (e) A simple contour generator converts the output voltage into a series of suitably spaced pulses which intensify the spot on a cathode ray oscillograph having a time-base raster synchronized with the rotation of the drum, thus providing the contours.

The following are the basic data pertaining to a computer capable of handling $h, k=\pm 12$ now under construction. The frequency of rotation of the drum is 1500 r.p.m. (25 cycles/sec.); the frequency of the basic sine wave (h=1) is 50 cycles/sec.). The time required for one complete scan of the x,y domain is about 20 sec., giving 1000 scanning lines. Provision has been made for altering the axial ratio, for oblique axes (by feeding part of the y-shift voltage into the x-plates of the C.R.O.), for ten co-ordinate lines on each axis, for distinguishing the negative contour levels and for automatic selection of any h,k recording for reading, erasing or changing the phase.

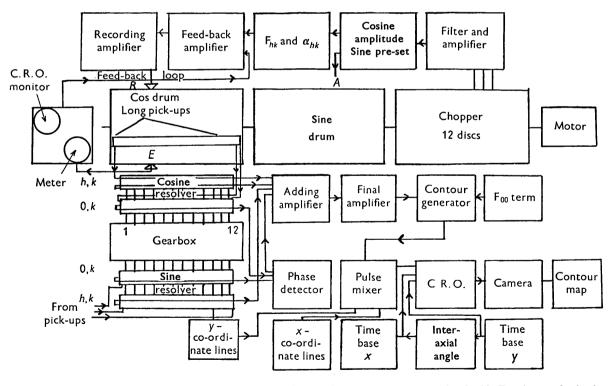


Fig. 1. Schematic block diagram of the synchronous magnetic recorder analogue computer for double Fourier synthesis. Arrows indicate the direction of the signal. R is the magnetic recording head and E is the pick-up head situated diametrically opposite to R. Both R and E are capable of moving to any position on the drums. For recording sine terms the lead marked A is switched into the recording channel in place of the cosine lead shown in position. Pick-ups similar to those shown on the cos drum are also on the sine drum. F_{hk} 's are set with the help of the meter. Appropriate filter circuits are selected by means of telephone uniselectors.

It is to be noted that the fundamental frequency has been chosen double that of the rotation of the drum so that in-phase signals can be picked off the diametrically opposite side to that of the recording side in order to get in-phase signals for applying negative feed-back. As only one set of indices, either h or k, need take negative values in problems relating to X-ray crystal-structure analysis if attention is confined to centrosymmetrical cases only, then a saving either in magnetic recording space or in the number of cosine resolvers can be effected by recording the cos terms with amplitudes $(F_{hk}+F_{-hk})$ and the sine terms with amplitudes $(F_{hk}-F_{-hk})$.

Because of their very low frequency, the axial terms of the type F_{0k} have to be dealt with on a different footing from the F_{h0} . They are also recorded on the drum with one of the basic frequencies with appropriate amplitudes, and subsequently passed through a separate set of cosine resolvers followed by a phase detector and then added in the final adding amplifier.

The following is a brief description of the contour generator employed. The output voltage from the computer is applied to one pair of plates of a short-persistence cathode ray tube. A set of suitably spaced slits is placed in front of the screen of the cathode ray tube and the light output falling on a photomultiplier gives electrical pulses which, suitably amplified and processed, give intensifying pulses to the grid of a second oscillograph whose time base is synchronized with the fundamental frequency and has a slow y-shift. The intensifying pulses occur whenever the output voltage crosses any of a set of pre-set voltage levels (as defined by the system of fine slits) and produces the contours.

A more elegant system based on generating the $\cos(hx\pm ky)$ signals directly by means of a set of pick-up heads moving coaxially with the magnetic recording drum has been designed and is eminently adapted not only for the production of direct Fourier synthesis but also for applying some of the more recent vector-shift and similar methods of crystal-structure analysis. Further description of the system is, however, deferred pending the construction of a computer based on this design. Recently Mohanti & Booth (1955) have devised a magnetic-recording type of Fourier synthesizer which, however, is different from the system described in the present paper.

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Données cristallographiques sur le cyanure de sodium hydraté: NaCN, 2H₂O. Par Hubert Curien et Thérèse Le Bihan, Laboratoire de Minéralogie-Cristallographie, Faculté des Sciences, Paris, France

(Reçu le 1 octobre 1956)

Formation

Par évaporation lente à température ordinaire d'une solution aqueuse de cyanure de sodium, on obtient des cristaux dont le degré d'hydratation a été précisé à l'aide de la thermobalance: il correspond à la formule NaCN, 2H₂O. Ces cristaux se déshydratent dès 40° C., se dissolvent dans leur eau d'hydratation et recristallisent sous la forme cubique stable à température ordinaire de NaCN anhydre.

Faciès

La symétrie est monoclinique. Le faciès est tabulaire avec {001} dominant. La plupart des cristaux se présentent sous forme de lames losanges limitées sur les cotés par {110} et {110}. On peut trouver aussi les faces {010}.

Maille cristalline

Les paramètres ont été déterminés sur des diagrammes de cristal tournant (radiation $Cu K\alpha$):

 $a = 6.08 \pm 0.01;$ $b = 10.66 \pm 0.01;$ $c = 6.54 \pm 0.01 \text{ Å};$ $eta=77^{\circ}~30'.$ $D_{
m exp.}=1{,}361~{
m g.cm.}^{-3};~~D_{
m calc.}=1{,}368~{
m g.cm.}^{-3};~~Z=4~.$

Les diagrammes de Weissenberg permettent de préciser le groupe.

Les extinctions systématiques observées sont: (h0l) pour h = 2n+1, et (0k0) pour k = 2n+1, compatibles avec le groupe P2₁/a. Un test de piézoélectricité s'est d'ailleurs avéré négatif.

Macle

Sur quelques échantillons, on a observé une macle par rotation autour de l'axe [001]. C'est une macle par pseudosymétrie, la maille commune aux deux individus étant une maille double.

Nous remercions M. J. P. Mathieu, Professeur à la Sorbonne, qui nous a signalé cette nouvelle forme hydratée et fourni les échantillons.