amplitudes, the binary digits (0 or 1) of the trigonometrical function (referred to below as the multiplier) serving only to give instructions to the tabulator. Fourteen binary digits are required to express one value of the function $10{,}000 \cos 2\pi nx$ (or $10{,}000 \sin 2\pi nx$), and each digit is represented on a card by a hole for 1 or a blank for 0. *Only one punching position is required to represent one binary digit* (so that since one column of 12 punching positions is required to represent one decimal digit for conventional arithmetical operations, about four ($\sim 12/\log_2 10$) times as much information can be carried on a card by the new method). Since the 14 digits of one particular multiplier are required to give 14 instructions in succession to the tabulator they are represented by the same punching position on 14 separate cards. The values of $\cos 2nx$ for a fixed value of n and values of x from 0 to $\frac{1}{4}$ at intervals of $\frac{1}{120}$, for example, are represented by 31 punching positions (less than 3 columns) on 14 cards. There is one such pack of 14 cards for each order n, and the appropriate value of the (three-figure) A_n is punched in the normal (decimal) way in the same columns on all 14 cards (negative amplitudes being punched as complements in four columns).

To carry out the summation $\overset{N}{\underset{0}{\Sigma}} A_n \cos 2\pi nx$ all the $14(N+1)$ cards are sorted into groups *in the order of the binary digits*. They are then tabulated in such a way that the amplitude is fed into the counter only if the corresponding binary digit on the card is 1. At the change of the binary digit, i.e. from the first to the second and so on, the contents of the counter are added to itself. Suppose in a very simple synthesis the data are as follows (the missing A_n's being all zero):

		Multiplier (e.g. $10 \sin 2nx_r$)				
n	A_n	Decimal		Bin	ary	
1	120	2	0	0	1	0
4	65	7	0	1	1	1
6	20	9	1	0	0	1
8	10	10	1	0	1	0
			a	b	c	d

The following tabulator operations are required to obtain $\Sigma A_n \sin 2\pi nx_r = 97 \cdot 5$:

(a)	Add $20+10$ into the counter and double	60
(b)	Add 65 and double again	250
(c)	Add $10+65+120$ and double again	890
(d)	Add $20+65$	975

In practice negative multipliers occur, and these may be dealt with either

(i) by adding 1 to all the sine and cosine values before converting to the binary scale, and subsequently making the necessary subtraction;

or (better)

(ii) by operating in the 'scale of minus two'. Any number, positive or negative, may be split into powers of -2, and the only change needed to multiply in this scale is to punch the amplitudes for alternate digits with signs reversed.

Since the data for each one-dimensional synthesis occupy only a few columns of the cards, the information for as many syntheses as convenient are punched into one pack of cards: for example, with 3-figure amplitudes and with syntheses extending over one-quarter of a cell side at $\frac{1}{120}$th intervals there is space for 18 one-dimensional syntheses. It is then possible, for example, at one passage of the same cards, to calculate the electron density at a number of points simultaneously *either* along the line (x, y_1, z_1) *or* along the line (x_r, y, z_1). This flexibility is of considerable value in exploring limited portions of an electron-density distribution.

We are indebted to Prof. E. G. Cox for providing facilities for this work and for his interest in it.

References

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Anomalous X-ray reflexions from copper crystals. By W. A. Rachinger, *Baillieu Laboratory, University of Melbourne, Australia*

In a recent investigation of the plastic properties of copper single crystals, it was found that when a deformed crystal was set in position for the high-angle (004) Co $K\alpha$ reflexion there sometimes appeared another line close to the main (004) reflexion. The relative position of this line and the (004) reflexion is shown in Fig. 1, which is a flat-film back-reflexion diagram. The extraneous line has a doublet structure and is not concentric with the (004) Debye circle. This latter fact rules out the possibility of the line being a primary Bragg reflexion due to radiation of another wave-length. It was also found that the reflexion was not a 'slit-effect' or due in any way to the experimental arrangement.

The line can, in fact, be shown to be due to a double reflexion of the incident X-ray beam, first by a ($1\bar{1}1$) and then by a ($\bar{1}13$) plane. This is illustrated by Fig. 2, which represents the trace of the (110) plane across the standard stereographic projection of a cubic crystal. The ($1\bar{1}1$), (001) and ($\bar{1}13$) poles are represented, not as points, but as circular areas since, as will be seen later, the double reflexion will accompany the primary (004) reflexion only in crystals which are imperfect in that their reflecting planes have a considerable orientation range. If the crystal is set so that the X-ray beam lies parallel to the (110) plane and is inclined at $8 \cdot 3°$ to the mean position of the (001) normals, then the direction of the beam will be represented by the point A in the standard projection. Now with the crystal in this position the (004) reflexion, for which $\theta = 81 \cdot 7°$, will take place and the direction of the reflected beam will be represented by the point B. The ($1\bar{1}1$) reflexion ($\theta = 25 \cdot 4°$) will also take place provided that the range of the ($1\bar{1}1$) normals is greater than $\pm 1 \cdot 6°$, since a point A' can then be found in the ($1\bar{1}1$) region which is $90 - \theta (= 64 \cdot 6°)$ from the incident beam A. The ray reflected from this plane A' will be represented by the point C. This ($1\bar{1}1$) reflexion can be further reflected by
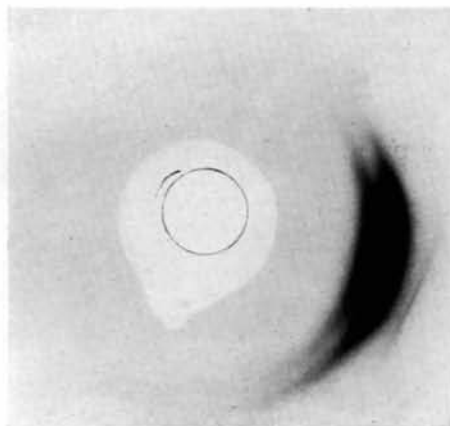
Fig. 1. The (004) and composite $(1\bar{1}1)+(\bar{1}13)$ reflexions from a deformed copper single crystal. The strong doublet ring is (004). The shorter, weaker, nearly straight line at 'four o'clock' outside the (004) ring is the double reflexion. The photograph was purposely over-exposed to show the double reflexion.

a ($\bar{1}13$) plane (provided that the angular range of ($\bar{1}13$) normals is greater than 1°), since there exists a ($\bar{1}13$) normal C' inclined at $90 - \theta (= 34\cdot9°)$ to the ($1\bar{1}1$) reflexion C. This composite ($1\bar{1}1$) and ($\bar{1}13$) reflexion has its direction represented by the point D which is inclined to the (004) reflexion B at an angle of $2\cdot4°$.
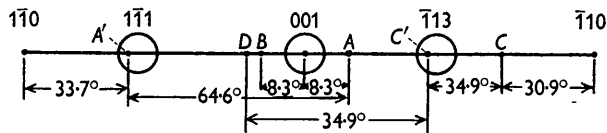

Fig. 2. A section of the standard stereographic projection of a cubic crystal (not to scale) showing the relative positions of the incident beam and reflected rays. A, incident beam; B, (004) reflexion; C, ($1\bar{1}1$) reflexion; D, the composite ($1\bar{1}1$)+($\bar{1}13$) reflexion.

Thus it can be seen that when a sufficiently imperfect copper crystal is set in an X-ray beam in the orientation indicated in Fig. 2 one obtains the primary (004) and ($1\bar{1}1$) Bragg reflexions and a double reflexion from the ($1\bar{1}1$) and ($\bar{1}13$) planes. This is illustrated in Fig. 3, which represents a section through the crystal parallel to the (110) plane.

Although the double reflexion (unaccompanied by the primary (004) reflexion) can be obtained with a perfect copper crystal, it can be detected more readily in the case of an imperfect crystal, since the variation in orientation of the reflecting planes allows a wider range of the setting angle at which the double reflexion will occur. In fact, under normal experimental conditions, the reflexion was frequently observed quite by chance. No unduly long exposures were required. The photograph of Fig. 1 had an exposure of 10 mA.hr. at 50 kV.

The foregoing description has been concerned only with the ideal case of a parallel beam and with reflexions and

reflecting normals parallel to the (110) plane, whereas in actual fact the reflexions will suffer considerable peripheral elongation due to the spread of the reflecting normals in a direction perpendicular to the (110) plane.
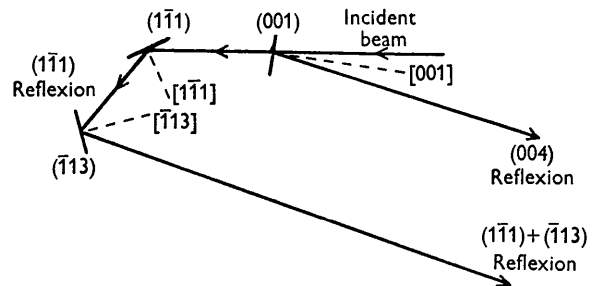

Fig. 3. A section through the crystal parallel to the (110) plane showing the primary and double reflexions.

The verification of the hypothesis of double reflexion was quite simple. The photograph shown in Fig. 1 was taken from a copper crystal which was set up in the orientation indicated by the point A of Fig. 2 and oscillated slightly about a mean position. The doublet separation of the double reflexion is equal to that of the ($\bar{1}13$) reflexion (the separation of the ($1\bar{1}1$) reflexion being negligible), whilst the minimum angular separation of the (004) reflexion and the double reflexion was approximately $2\cdot4°$, which is consistent with the angular separation of the points B and D of Fig. 2.

In conclusion, the author wishes to thank Dr W. A. Wood of the Baillieu Laboratory, University of Melbourne, and Dr A. Matheson of the Division of Industrial Chemistry, C.S.I.R.O., for their interest and helpful advice.

β-Diglycylglycine.[†] By Edward W. Hughes and Walter J. Moore[‡], *Gates and Crellin Laboratories, California Institute of Technology, Pasadena, California, U.S.A.*

In a brief survey examination Lenel (1932) has reported unit-cell data for two anhydrous forms of diglycylglycine. His constants for the β-form are:

monoclinic, $a = 14\cdot6$, $b = 4\cdot79$, $c = 11\cdot67$ kX.; $\beta = 105\frac{1}{2}°$.

There are four molecules per cell. No space group was given, and the measurements were made on rotation and Weissenberg photographs taken about the needle axis, b.

We have grown needle-like crystals of diglycylglycine by slowly cooling a saturated 40% aqueous ethanol solution of the substance. After preparing rotation and zero-layer Weissenberg photographs about the needle axis we found, assuming monoclinic symmetry, constants which agree with Lenel's within experimental error:

$a = 14\cdot92$, $b = 4\cdot80$, $c = 11\cdot67$ kX.; $\beta = 105°$,

and it seems probable that we had the form he called β. However, these needles show oblique extinction between

crossed Nicol prisms, and Laue photographs taken perpendicular to the needle axis in various orientations show no symmetry planes. A first-layer Weissenberg picture about the needle axis confirms that the Laue symmetry is $\bar{1}$ and that the crystal is grossly triclinic. Although it is barely possible that we have discovered a third form of diglycylglycine it seems more likely that Lenel erred in calling the β-form monoclinic.

The cell is simple and contains four molecules so that even if the space group is $P\bar{1}$ there are two non-equivalent molecules per cell; if the space group is $P1$ there are four non-equivalent molecules. It is therefore an unfavorable substance for detailed examination and we have abandoned it. It should be noted that we have not determined the crystal angles α, β and γ, and the proper constants to be recorded in place of those above are:

$d_{100} = 14\cdot41$, $b = 4\cdot80$, $d_{001} = 11\cdot27$ kX.; $\beta^* = 75°$.

We are indebted to Prof. Eugene Pacsu for the sample of diglycylglycine.

Reference

Lenel, F. V. (1932). *Z. Krystallogr.* **81**, 224.