Table 2 (*cont.*)

hkl	$F_{obs.}$	$F_{calc.}$	α (°)
512	8·0	8·3	344
522	5·9	5·6	26
532	5·3	3·4	123
542	5·7	5·0	338
552	6·5	5·7	338
562	3·8	4·3	107
572	4·4	4·3	285
582	2·7	2·9	299
592	2·2	2·8	88
5,10,2	1·5	1·9	101
503	—	1·1	270
513	6·4	4·6	205
523	2·6	3·6	264
533	11·7	12·3	171
543	2·9	3·4	42
553	—	2·3	348
563	3·2	3·4	264
504	—	0·4	180
514	2·7	2·1	238
524	3·4	3·2	338
534	2·9	2·4	120
544	—	0·7	23
600	2·7	1·4	180
610	7·7	6·6	270
620	5·1	3·9	0
630	1·2	1·2	90
640	1·0	3·0	0
650	7·5	8·2	270
660	5·2	6·8	180
670	6·7	5·7	270
680	2·9	1·6	180
690	1·1	0·7	270
6,10,0	—	0·1	180

hkl	$F_{obs.}$	$F_{calc.}$	α (°)
6,11,0	5·9	5·9	270
601	0·9	0·2	270
611	2·3	1·2	197
621	5·3	3·1	80
631	3·0	2·3	112
641	4·9	5·7	355
651	2·0	2·5	15
661	5·1	3·9	86
671	2·6	2·4	138
681	2·0	2·6	355
691	4·3	3·6	348
6,10,1	1·7	2·3	113
602	9·2	10·6	180
612	9·0	8·5	237
622	1·9	2·3	17
632	2·9	1·7	327
642	3·2	3·0	257
652	6·7	7·0	233
662	3·9	3·8	161
672	3·7	3·9	264
682	2·7	4·1	332
603	5·0	5·1	90
613	2·7	2·7	302
623	0·8	0·9	201
633	4·1	4·2	17
643	2·9	2·8	103
653	2·2	2·6	205
604	2·9	3·4	180
614	4·2	4·0	303
700	8·1	8·3	180
710	2·5	1·2	270

hkl	$F_{obs.}$	$F_{calc.}$	α (°)
720	0·9	0·2	0
730	2·1	2·2	270
740	3·8	3·0	180
750	—	1·3	90
760	1·4	0·2	0
770	—	0·7	270
780	1·8	0·7	0
701	5·1	6·7	90
711	3·8	3·6	316
721	6·7	6·4	259
731	3·9	3·9	6
741	4·0	3·5	213
751	2·7	2·1	316
761	1·1	2·3	114
771	1·7	1·2	269
781	3·5	4·5	249
702	0·7	0·8	180
712	2·6	1·1	168
722	1·3	1·3	6
732	3·4	3·1	26
742	1·7	2·0	90
703	1·0	0·7	270
713	1·3	1·0	162
800	6·5	4·3	0
810	1·1	0·8	90
820	1·4	1·9	0
830	2·1	2·4	90
801	3·0	2·3	90
811	3·2	2·8	88
821	3·9	1·3	299

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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A new punched-card method of Fourier synthesis.

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In the Hollerith methods for summing Fourier series which have been described hitherto (e.g. Cox, Gross & Jeffrey, 1947) the punched cards have been essentially more accurate Beevers–Lipson strips. It was possible to reduce the number of cards by using the technique of 'progressive digiting', and subsequently we found that further advantages could be obtained by expressing the amplitudes in the binary scale and using the feature of the B.T.M. Rolling Total Tabulator whereby a counter can be added into itself to double its contents; nevertheless, all methods retained an undesirable feature of the original Beevers–Lipson procedure, namely, the preliminary selection of cards from a filing system. Hand selection requires careful checking, and ultimately the cards must be refiled and again checked; these are tedious and time-consuming operations, however well they are organized.

This note outlines the principles of a new method which has been developed by one of us (D. M. S. Greenhalgh) and which has the great advantage that hand selection and filing of cards have been eliminated. Full technical details are being published elsewhere (Greenhalgh, 1950). For the first stage of a synthesis, the appropriate amplitudes A_n are hand-punched on to the relatively small number of cards required, and for subsequent stages the amplitudes can be summary-punched from the results of the preceding summations. The trigonometric functions are represented in the binary scale in the way described below, and are transferred to these cards from a master pack. The whole set of cards can be stored afterwards as a compact and permanent record of the job.

All the arithmetical operations in a synthesis by the new method are performed in the ordinary decimal scale on the 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 $\sum_0^N A_n \cos 2\pi nx$ 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 $2\pi nx_r$)				
n	A_n	Decimal	Binary			
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.

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Anomalous X-ray reflexions from copper crystals.

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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