REMARKS ON A PAPER OF PÁL MEDGYESSY: "A MECHANICAL FUNCTIONAL SYNTHESIZER"

by

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I.

The mechanical functional synthesizer planned by P. MEDGYESSY[2]) and operating in our Department has been used to calculate the projection of electron density in crystals.

Since the electron density in a crystal as well as its projection on a plane are periodical functions of the coordinates, they can be calculated by means of Fourier series [2]. By calculating the electron density in three dimensions one makes use of a three-dimensional series (with three sets of indices denoted by h, k and l while in projection the series is reduced to a two-dimensional one (one of the indices, say h being zero). Let us take for example the cristallographic axis x as the direction of projecting and project the unit cell on the yz plane. Supposed the crystal has a center of inversion, the projection of the electron density can be described in this case by the following Fourier series:

$$(1) \quad \varrho'(yz) = \frac{1}{A} \sum_k \sum_l F(0\,kl) \cos 2\pi(ky + lz) = \frac{1}{A} \sum_k \sum_l F(0\,kl) \cos (k\alpha + l\beta).$$

Notations:

A = the area of the projection

k, l = integers, indices of the series (corresponding to the "Miller indices" used in crystallography)

$F(0kl)$ = the coefficiens of the series, which are identical with the "structure factors" of the crystallographic planes with Miller indices: $(0kl)$. This quantities can be measured on X-ray diffraction photographs.

y, z = relative coordinates referred to the length of the corresponding edge of the unit cell.

$\varrho'(yz)$ = electron density measured in units: number of electrons per square Ångström.

$\alpha = 2\pi y$

$\beta = 2\pi z$

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[2]) Pál Medgyessy: "A Mechanical Functional Synthesizer" *(Publications of the Mathematical Institute of the Hungarian Academy of Science.* **2** (1957) 33—42.)

This two-dimensional synthesis can be reduced to two successive one-dimensional ones by means of a simple trigonometric subtitution (For sake of simplicity we introduce the notation : $\varrho(yz) = A\varrho'(yz)$

$$(2) \quad \varrho(yz) = \sum_k \left[\sum_l F(0\,kl) \cos l\beta\right] \cos k\alpha - \sum_k \left[\sum_l F(0\,kl) \sin l\beta\right] \sin k\alpha \ .$$

Introducing for the results of the first summation the notation :

$$S_1(k,z) = \sum_l F(0\,kl) \cos l\beta\,; \qquad S_2(k,z) = \sum_l F(0\,kl) \sin l\beta$$

and writing the constant terms of the series : F (000) and $S_0 = S_1\ (o, z)$ separately :

$$(3) \qquad \varrho(yz) = F(000) + S_0 + \sum_{\substack{k \\ k\neq 0}} \left[S_1(k,z) \cos k\alpha - S_2(k,z) \sin k\alpha\right] \ .$$

Since we want to work with the mechanical synthesizer we have to keep in mind that it has patterns of the form

$1 \pm \sin k\lambda$ resp. $1 \pm \cos k\lambda$ and it can synthesize terms like :

const. $(1 \pm \sin k\lambda) \cdot$ resp. const. $(1 \pm \sin k\lambda)$

where the constant factor is always positive. So it is comfortable for us to transform our equation :

$$(4) \qquad \begin{aligned} \varrho(yz) = \sum_{\substack{k \\ k\neq 0}} &[|\,S_1(k,z)| + S_1(k,z) \cos k\lambda + |\,S_2(k,z)| - S_2(k,z) \sin k\alpha\,] - \\ &- \Big\{\sum_{\substack{k \\ k\neq 0}} [|S_1(k,z)| + |\,S_2(k,z)|\,] - F(000) - S_0.\Big\} \end{aligned}$$

Introducing the notation :

$$\Sigma = \sum_{\substack{k \\ k\neq 0}} [|\,S_1(k,z)| + S_1(k,z) \cos k\alpha + |\,S_2(k,z)| - S_2(k,z) \sin k\alpha\,]$$

$$C = \sum_{\substack{k \\ k\neq 0}} [|\,S_1(k,z)| + |\,S_2(k,z)|\,] - F(000) - S_0$$

we obtain the equation

$$(5) \qquad \varrho(yz) = \Sigma - C$$

from which it is obvious that *the projection of the electron density* $\varrho(yz)$ *is obtained by subtracting the constant term* C *from the value* Σ *indicated by the mechanical synthesizer.*

The result of a summation appears on the instrument as end-points of bars, in 37 equidistant points having the values $0 < \alpha < \pi$; in our case, this sum corresponds to the projection of the electron density along a line $z =$ constant and $0 < y < \frac{1}{2}$. (see the paper of P. MEDGYESSY [1].)

At first time, after having read the positions of the end-points of bars on a scale fixed under the bars, we wrote the date on an yz net. After this

we put a transparent paper over the net and traced the lines of equal electron density in order to find the maxima, that is the places of atomic centers.

In order to speed up our work we have initiated a new method for fixing the results of the second summation. Instead of reading, we draw the sum on a leaf of drawing-paper : First, we trace a straight line on the paper then we put the paper between the bars and the scale so that the straight line coincided with the value

$$C = \sum_{\substack{k \\ k \neq 0}} \left[|S_1(k,z)| + |S_2(k,z)| \right] - F(000) - S_0 ,$$

then we mark the end of each bar and cut the figure we have got in this way. Such a figure corresponds to the projection of the electron density along a line $z = \text{const.}$ and $0 < y < \frac{1}{2}$. As we have calculated the first sums $S_1(k,z)$ and $S_2(k,z)$ in equidistant points of the z axis, we shall have now as many figures as z values.

We constructed a square frame for the figures and mounted them into the inner slits of the frame. The figures were arranged according to their z values, while the O lines of each figure were held in equal height. So we obtained a very clear three dimensional representation of the function $\varrho(yz)$ (Fig. 1.). Two horizontal directions correspond here to the y resp. z axis and the vertical direction to $\varrho(yz)$. The maxima are immediately observable and their coordinates and height could be read on a scale made of plexiglass.

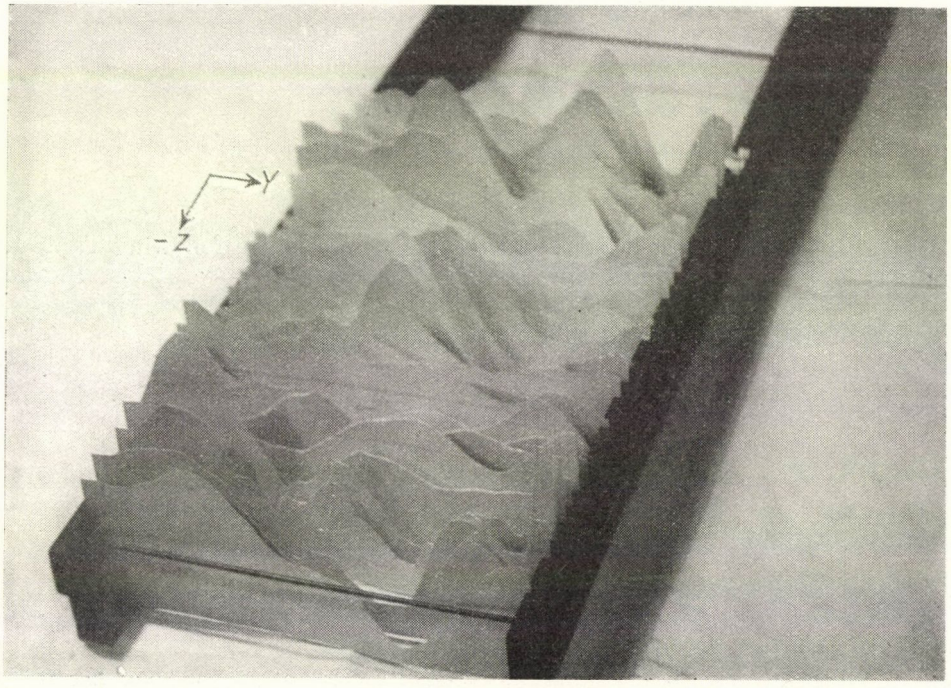

Figure 1.

The main advantage of the new method beside its graphic character is, that it reduces the working time. With the old method the calculations took up scarcely less time than with the BEEVERS—LIPSON strips. Now we work three times faster and we do not need drawing an electron density map.

II.

As mentioned in section I. the instrument has patterns of the shape $1 \pm \sin k\alpha$ and $1 \pm \cos k\alpha$. The values on the patterns are calculated in steps of 5 degrees and also the sum is obtained in these points. In the course of crystal structure work, in case of a large unit cell, there occur indices of 30—40 and even larger ones. It is easy to show that the preparing of the patterns is needed only up to $k = 18$ and patterns with $k > 18$ can be substituted by patterns with $k < 18$, *supposed we want to obtain the results in the mentioned equidistant points of 5 degrees.*

It is suitable to introduce the following notation: We denote "pattern $\sin k_i$" and "pattern $\cos k_i$" the patterns of the shape $1 + \sin k_i$ and $1 + \cos k_i$ further "pattern $-\sin k_i$" and "pattern $-\cos k_i$" the patterns of the shape $1 - \sin k_i$ resp. $1 - \cos. k_i$. As "even steps" are denoted the steps $\alpha = 2n5°$ of the patterns and as "odd steps" those of $\alpha = (2n + 1)\,5°$. We shall use the name "even bars" and "odd bars" for the bars shifted by the even resp. odd steps of the patterns.

Keeping in view that we calculate in steps of 5 degrees and that the values of the trigonometric functions of arguments larger than 90 degrees can be substituted by values belonging to arguments less than 90 degrees, we can fit together following relations:

$$a)\ \sin[(2n+1)(36-k)\,5°] = \sin[(2n+1)\,k\,5°]$$

$$b)\ \sin[2n(36-k)\,5°] = -\sin(2n\,k\,5°)$$

$$c)\ \cos[(2n+1)(36-k)\,5°] = -\cos[(2n+1)\,k\,5°]$$

$$d)\ \cos[2n(36-k)\,5°] = \cos(2nk\,5°).$$

Making use of the previous and similar relations the following Table I. can be prepared. This table shows the sign relationship between $k > 18$ and the substituting patterns $k < 18$.

Table I

	α	k	I $36 - k$	II $k - 36$	III $72 - k$
Sin	$(2n+1)\cdot 5°$	+	+	−	−
	$2n \cdot 5°$	+	−	+	−
Cos	$(2n+1)\cdot 5°$	+	−	−	+
	$2n \cdot 5°$	+	+	+	+

The column I. is to be used if $18 \leqq k \leqq 36$; column II. if $36 \leqq k \leqq 54$ and column III. if $54 \leqq k \leqq 72$. (The case $k > 72$, has no practical significance.)

We can elucidate the use of the Table on an example : It is to be added $S_2(21, z)$. sin 21 α. From the table it is clear that instead of the pattern sin 21 we must apply pattern sin 15 for the odd steps, and pattern $-$sin 15 for the even steps. In practice this can be achieved by putting pattern sin 15 into the instrument and shift forward so that only the odd bars moved and the even ones remained in their original positions. After this we put in pattern $-$sin 15 and now we must be able to set in motion only the even bars and leave the others unmoved.

Our instrument is built so that the bars can move only together. We must transform the instrument so that the even bars and the odd bars could move either seperately or together. By a slight modification this can be done but the description of the technical details exceed the scope of this communication.

We have to treat particularly the function: cos 36 α. It has values $+1$ at $\alpha = 2n \cdot 5°$ and -1 at $\alpha = (2n + 1) \cdot 5°$. According to our notation in section I. its coefficient is $S_1(36, z)$ and the value of the function $S_1(36, z)$ cos 36 is at the even steps equal to $S_1(36, z)$ and at the odd steps : $-S_1(36, z)$. According to Table I. we need the pattern cos 0 for its addition to the series. This pattern has been eliminated by including his coefficient S_0 into the constant term C (equation 5. in section I.), therefore it would be necessary to prepare pattern cos 36 as the unique one from among the patterns $k > 18$. Still there is a simple way to avoid this, by including also this term into the constant term of the addition. In practice this can be performed in the following way : After having added all the terms included in Σ (equation [5], section I.) we put our leaf of paper under the bars so that the $\varrho(yz) = 0$ line coincided with the value $C' = C - S_1(36, z)$ of the scale and mark the endpoints of the even bars. After this, we shift the O line to the value $C'' = C + S_1(36, z)$ and now we mark the positions of the odd bars.

It has to be mentioned that the Beevers—Lipson strips applied in crystal structure analysis are constructed on the basis of similar ideas. Here, the values of the trigonometric functions are printed on both sides of a strip of paper, in intervals of 3 degrees. The values belonging to the even multiples of 3 degrees are on one side and those belonging to the odd multiples on the other side.

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REFERENCES

[1] MEDGYESSY P. : "A Mechanical Functional Synthesizer". *Publ. of the Mathematical Institute of the Hungarian Academy of Science.* **2** (1957) 33—42.

[2] LIPSON, H.—COCHRAN, W. : *The Determination of Crystal Structures.* The Crystalline State Vol. III. London 1953.

MEGJEGYZÉSEK MEDGYESSY PÁL: „EGY MECHANIKAI FÜGGVÉNYSZINTETIZÁTOR" CÍMŰ CIKKÉHEZ

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Kivonat

Medgyessy Pál [1] cikkében leírt szintetizátorral számoltunk. A számolási időt kb. harmadára csökkentettük azáltal, hogy az eredményeket nem olvastuk le, hanem a pálcák alá karton papírost téve megjelöltük a pálcák végpontjait és az így kapott ábrát kivágtuk. Az ábrákat egymás mellé rakva az elektronsűrűség vetületi eloszlásának szemléletes, háromdimenziós képe alakult ki.

Kimutatjuk, hogy a sablonok $h = 18$-ig való elkészítésével az összegezési lehetőséget bármilyen magas frekvenciáig ki lehet terjeszteni. Ez által a sablonok költséges elkészítését megtakaríthatjuk.

ЗАМЕЧАНИЯ К СТАТЬЕ P. MEDGYESSY: „ОДИН МЕХАНИЧЕСКИЙ ФУНКЦИОНАЛЬНЫЙ СИНТЕТИЗАТОР"

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Резюме

Мы считали с помощью синтетизатора, описанного в статье P. Medgyessy [1]. Мы сократили время счёта примерно в три раза следующим образом: мы не читали результаты, а, положив под палочки картон, отметили концы палочек и вырезали полученный чертёж. Поместив рядом полученные чертежи, мы получили наглядную, трёхмерную картину проекционного распределения плотности электронов.

Мы показываем, что изготовляя шаблоны до $h = 18$ возможность суммирования может быть распространена до как угодно высокой частоты. Таким образом мы можем съэкономить дорогостоящее изготовление шаблонов.