the $Cr^{3+}$ ions, which increases from $NaCrSe_2$ to $RbCrSe_2$, following the decreasing contrapolarizing action of the ions in the series $Na^+$—$Rb^+$.

Table 3. *Observed and calculated interionic spacings of the alkali selenochromites*

(All values in A.)

| Spacing | | $NaCrSe_2$ Obs. | $NaCrSe_2$ Calc. | $K_{0.5}CrSe_2$ Obs. | $K_{0.5}CrSe_2$ Calc. | $RbCrSe_2$ Obs. | $RbCrSe_2$ Calc. |
|---|---|---|---|---|---|---|---|
| Alk.–Se | | 2·92 | 2·89 | 3·27 | 3·24 | — | 3·40 |
| Cr–Se | | 2·55 | 2·55 | 2·46 | 2·55 | — | 2·55 |
| Cr–Cr | within one layer | 3·70 | — | 3·44 | — | 3·43 | — |
| Se–Se | within one layer | 3·70 | 3·82 | 3·44 | 3·82 | 3·43 | 3·82 |
| Alk.–Alk. | within one layer | 3·70 | — | 3·44 | — | 3·43 | — |

The mobility of the electrons of the selenium ions, which increases with the polarization, is manifested in the electric conductivity of the compounds. While $NaCrS_2$ is still nearly a non-conductor, the specific resistance measured on samples under a pressure of 1200 kg.cm.$^{-2}$ is 6·4 ohm-cm. for $NaCrSe_2$ and 0·2 ohm-cm. for $RbCrSe_2$. The conductivity of $RbCrSe_2$ is thus not much less than that of microcrystalline graphite.

In Table 3 the observed interionic spacings of the alkali selenochromites are compared with the values calculated from the Goldschmidt ionic radii.

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# Indexing Powder Photographs of Tetragonal, Hexagonal and Orthorhombic Crystals

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(*Received* 8 *March* 1948)

A numerical method of indexing X-ray powder photographs without the use of single-crystal data is described. The method leads to a fairly systematic treatment of tetragonal and hexagonal photographs, and has also proved valuable in orthorhombic cases.

The indexing of powder photographs of tetragonal and hexagonal materials, which cannot be obtained in suitable single crystals, is most frequently carried out by means of the graphical methods of Hull & Davey (1921), Bjurström (1931), and of Bunn (1945, p. 133). These and other related graphical methods are, however, very time-consuming and are liable to fail in cases with a high proportion of missing reflexions. Some crystallographers might prefer to solve the problem numerically if practicable methods existed. The early numerical methods of Runge (1917) and of Johnsen & Toeplitz (1918), however, are mainly of theoretical interest and will generally not work in practice.

In the following, an account is given of a numerical method which has proved to be very successful in several practical tests carried out in Uppsala. It allows of a fairly systematic treatment of tetragonal and hexagonal cases. It has also been successful in ortho rhombic cases, although there the treatment will be less systematic. Earlier investigators may have applied similar methods to those of this paper, but a consistent account seems to be lacking.

## 1. TETRAGONAL AND HEXAGONAL (RHOMBOHEDRAL) SYSTEMS

### 1·1. General relations

In the tetragonal and hexagonal (rhombohedral) systems the quadratic forms are

$$\sin^2\theta = \frac{\lambda^2}{4}\left(\frac{h^2+k^2}{a^2}+\frac{l^2}{c^2}\right)$$

and

$$\sin^2\theta = \frac{\lambda^2}{4}\left(\frac{4(h^2+k^2+hk)}{3a^2}+\frac{l^2}{c^2}\right),$$

with well-known notations. We introduce the following notations:

| | Tetragonal system | Hexagonal system |
|---|---|---|
| $A =$ | $\lambda^2/(4a^2)$ | $\lambda^2/(3a^2)$ |
| $C =$ | $\lambda^2/(4c^2)$ | $\lambda^2/(4c^2)$ |
| $M =$ | $(h^2+k^2)$ | $(h^2+k^2+hk)$ |
| | ('tetragonal number') | ('hexagonal number') |

and further $q=\sin^2\theta$.* All these quantities are positive. We can then write for both the tetragonal and hexagonal system

$$q=AM+Cl^2,$$

where for the tetragonal system $M=0, 1, 2, 4, 5, 8$, etc., and for the hexagonal system $M=0, 1, 3, 4, 7, 9$, etc.

If a number of $q$ values are given, the problem will be to solve the system of equations

$$q_i=M_iA+l_i^2C \quad (i=1,\ 2,\ 3, \text{ etc., } q_i \text{ given})$$

with respect to $A$, $C$, $M_i$ and $l_i^2$, establishing the simplest possible solutions.

Let us represent $p=NA+RC$, where $N$ and $R$ are integers, by a number pair $(p)=(N, R)$, for which the following calculation rules are defined (cf. the calculation rules for complex numbers):

(*a*) $(N_1, R_1)=(N_2, R_2)$, only if $N_1=N_2$ and $R_1=R_2$;

(*b*) $\Sigma k_i(N_i, R_i)=(\Sigma k_iN_i, \Sigma k_iR_i)$, where $k_i$ are integers.

If the representation is not unique, that is, if $p=N'A+R'C=N''A+R''C$, where $N'\neq N''$, we still write $(N', R')\neq(N'', R'')$.

It is seen that if $\Sigma k_i(p_i)=(0, 0)$, then

$$\Sigma k_iN_i=0 \quad\text{and}\quad \Sigma k_iR_i=0.$$

Now let $q$ be represented by the number pair

$$(q)=(M, l^2).$$

In the following we consider only lines with fairly small $q$ values, i.e. lines with fairly small values of $M$ and $l^2$. It is also assumed that $A:C$ is not a ratio of small or relatively small integers. Then the representation $(q)=(M, l^2)$ is unique. (For if $q=M_1A+l_1^2C=M_2A+l_2^2C$, then $A:C=(l_2^2-l_1^2):(M_1-M_2)$.)

Also if $\sum^n k_iq_i=0$ ($k_i$=small positive or negative integers; $n$ small, generally $\leqq 4$), then $\sum^n k_i(q_i)=(0, 0)$. (If this is not valid, then $A:C=(-\sum^n k_il_i^2):(\sum^n k_iM_i)$, which is in conflict with the assumption.) If then relations of the type $\sum^n k_iq_i=0$ have been found by the method explained in § 1·3, $M_i$ and $l_i^2$ can be calculated from the corresponding equations

$$\left(\sum^n k_iM_i, \sum^n k_il_i^2\right)=(0, 0).$$

* If one prefers a function which is independent of $\lambda$, one may replace $q$ in all the following expressions by

$$Q=4\ (\sin^2\theta)/\lambda^2.$$

The meaning of the constants $A$ and $C$ will then change to $A=1/a^2$ (tetragonal system), $A=4/(3a^2)$ (hexagonal system), and $C=1/c^2$.

*Linear relation between two q values*

Of special interest are equations of the type

$$k_1q_1=k_2q_2$$

and of the type

$$k_1q_1+k_2q_2+k_3q_3=0.$$

We first consider the equation $k_1q_1=k_2q_2$, where $k_1$ and $k_2$ possess no common factor and where $k_1$ and $k_2$ are not both squares.

Then $(k_1M_1,\ k_1l_1^2)=(k_2M_2,\ k_2l_2^2)$, from which $M_1:k_2=M_2:k_1$ and $k_1l_1^2=k_2l_2^2$.

From this it follows that $l_1=l_2=0$. For assume $l_1\neq 0$ which implies $l_2\neq 0$, then $l_2$ must contain all the prime factors of $k_1$, and $l_1$ must contain all the prime factors of $k_2$. If then $k_1$, say, is not a square, it must contain a prime factor $p$ to an odd power. In this case $l_2$ must contain the factor $p$, which will then enter to an even power in the right-hand member of $k_1l_1^2=k_2l_2^2$, while the left-hand member contains $p$ to an odd power. Consequently, the assumption $l_1\neq 0$ leads to a paradox.

We thus find that $(q_1)=(M_1, 0)$ and $(q_2)=(M_2, 0)$ and further $M_1:k_2=M_2:k_1=m_{12}$ ($m_{12}$=an integer $\geqq 1$ because $k_1$ and $k_2$ have no common factor).

Hence $A=\dfrac{q_1}{M_1}=\dfrac{1}{m_{12}}\dfrac{q_1}{k_2}$, where $q_1$ and $k_2$ are known.

If $m_{12}>1$ one can often find $m_{12}$ or factors in $m_{12}$ by the combination of several equations. As an example, we consider the following equations:

$$(1)\ q_1=3q_2, \qquad (2)\ q_1=4q_3.$$

Then

(1) gives $(q_1)=(3M_2, 0)$ and (2) gives $(q_1)=(4M_3, 4l_3^2)$, where evidently $l_3=0$. (1) also gives $A=\dfrac{1}{m_{12}}\dfrac{q_1}{3}$. Here $m_{12}=M_2$. But as $(3M_2, 0)=(4M_3, 0)$, it follows that $3M_2=3m_{12}=4M_3$, i.e. $m_{12}$ must contain the factor 4. As a consequence $A=q_1/(12m)$, where $m$=an integer, possibly 1.

The ratio $k_2:k_1=M_1:M_2$ generally determines whether the system is tetragonal or hexagonal. The occurrence of the simplest ratios in these two systems is tabulated in Table 1.

Table 1. *Occurrence of ratio $M_1:M_2$ (expressed in numbers $<10$) without a common factor in tetragonal ($T$) and hexagonal ($H$) systems. The ratios denoted by* 0 *do not occur*

| | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|
| 1 | *T* | *H* | *TH* | *T* | 0 | *H* | *T* | *TH* |
| 2 | | 0 | — | *T* | — | 0 | — | *T* |
| 3 | | | *H* | 0 | — | *H* | 0 | — |
| 4 | | | | *T* | — | *H* | — | *TH* |
| 5 | | | | | 0 | 0 | *T* | *T* |
| 6 | | | | | | 0 | — | — |
| 7 | | | | | | | 0 | *H* |
| 8 | | | | | | | | *T* |

*Linear relation between three q values*

The equation $k_1q_1+k_2q_2+k_3q_3=0$ gives

$$(k_1M_1+k_2M_2+k_3M_3,\ k_1l_1^2+k_2l_2^2+k_3l_3^2)=(0, 0).$$

The equation $k_1 l_1^2 + k_2 l_2^2 + k_3 l_3^2 = 0$ has very few solutions which are small numbers. The equation

$$2l_1^2 + 2l_2^2 - l_3^2 = 0$$

for example, has for $0 \leqq l_i < 10$ only solutions of the form $l_1 = l_2 = n$, $l_3 = 2n$. Solutions to equations of this kind are given in Table 2 for

$$|l_i| < 10 \quad \text{and} \quad |k_1| \leqq 6, \quad |k_2| \leqq 3, \quad |k_3| \leqq 3.$$

The solution $l_1 = l_2 = l_3 = 0$ is common to all equations of this type. This solution implies that

$$q_1 : q_2 : q_3 = M_1 : M_2 : M_3.$$

Hence this solution is excluded except when $q_1$, $q_2$ and $q_3$ stand in such a rational proportion. If

$$q_1 : q_2 : q_3 = k_1 : k_2 : k_3,$$

where $k_i$ = integers without a common factor and one of the $k_i$ is non-quadratic, then $A = q_1/(mk_1)$, where $m$ is an integer.

By combining several equations $k_1 l_1^2 + k_2 l_2^2 + k_3 l_3^2 = 0$ with equations $k_i q_i = k_j q_j$ or $\sum^4 k_i q_i = 0$ it is possible to calculate $l_i$ for a number of lines (see § 1·4, example 2). In this way one obtains

$$A = (l_2^2 q_1 - l_1^2 q_2)/n_{12} = (l_3^2 q_1 - l_1^2 q_3)/n_{13} = (l_4^2 q_1 - l_1^2 q_4)/n_{14}$$

and so on, where $n_{12}$, $n_{13}$, $n_{14}$ are integers. If $l_i$ and $l_j$ have the common factor $k$, then $n_{ij}$ contains the factor $k^2$. (In these expressions it is assumed that

$$l_j^2 q_i - l_i^2 q_j \neq 0.)$$

By combining several equations $\sum^3 k_i M_i = 0$ with, possibly, equations $k_i M_i = k_j M_j$ or $\sum^4 k_i M_i = 0$, one also obtains possible solutions in $M$. In this way one can obtain possible values for $m_{ij} = M_i l_j^2 - M_j l_i^2$.

### 1·2. Determination of one constant when the other is known

The treatment of this problem does not imply any new features, but is briefly related here for the sake of completeness.

If $(q) = (M, l^2)$ then $(q - AM) = (0, l^2)$. Thus, if $q$ is a reflexion with unknown indices, one of the numbers $q - M_i A$ ($\geqq 0$; $M_i = 0$, 1, 2, 4, 5, etc. in the tetragonal system and $= 0$, 1, 3, etc. in the hexagonal system) will equal $Cl^2$.

If $A$ is given and one knows whether the system is tetragonal or hexagonal, one selects the four or five lowest $q$ values for which $(q) \neq (M, 0)$ and forms $q_i - AM_j > 0$, where $M_j$ are either tetragonal or hexagonal numbers. If the system is unknown, both tetragonal and hexagonal numbers are given to $M_j$. If among the reflexions in question ($q_1 < q_2 < q_3 < q_4 < q_5$) two, for instance $q_1$ and $q_3$, possess the same $l$ index, then

$$q_1 - M_1 A = q_3 - M_3 A = k_c, \quad \text{where} \quad k_c = Cl^2.$$

Table 2. *Solutions* $0 \leqq l_i < 10$ *of the equation* $k_1 l_1^2 + k_2 l_2^2 + k_3 l_3^2 = 0$, *for* $|k_1| \leqq 6$, $|k_2| \leqq 3$, $|k_3| \leqq 3$

(Equation $k_1 l_1^2 + k_2 l_2^2 + k_3 l_3^2 = 0$ is identical with $-k_1 l_1^2 - k_2 l_2^2 - k_3 l_3^2 = 0$.)

General solution: $l_1 = l_2 = l_3 = 0$.

Type solutions: (*a*) $k_1 + k_2 + k_3 = 0$; $l_1 = l_2 = l_3$.
(*b*) $k_i = -k_j$; $l_i = l_j$, $l_s = 0$.
(*c*) $k_i = -4k_j$; $2l_i = l_j$, $l_s = 0$.

| Coefficients | | | Type solutions (see above) | Special solutions | | |
|---|---|---|---|---|---|---|
| $k_1$ | $k_2$ | $k_3$ | | $l_1$ | $l_2$ | $l_3$ |
| 1 | −1 | −1 | *b*, *b* | 5<br>5 | 4<br>3 | 3<br>4 |
| 2 | 1 | −1 | *b* | $2n$<br>4 | $n$<br>7 | $3n$<br>9 |
| 2 | −1 | −1 | *a* | 5<br>5 | 7<br>1 | 1<br>7 |
| 2 | 2 | −1 | — | $n$ | $n$ | $2n$ |
| 2 | −2 | −1 | *b* | $3n$<br>9 | $n$<br>7 | $4n$<br>8 |
| 3 | 1 | −1 | *b* | $n$<br>4 | $n$<br>1 | $2n$<br>7 |
| 3 | −2 | −1 | *a* | 3 | 1 | 5 |
| 3 | 2 | −2 | *b* | 4<br>4 | 1<br>5 | 5<br>7 |
| 3 | −3 | 1 | *b* | $n$ | $2n$ | $3n$ |
| 3 | −3 | 2 | *b* | 1<br>5 | 5<br>7 | 6<br>6 |
| 4 | 1 | −1 | *b*, *c* | 2 | 3 | 5 |
| 4 | −1 | −1 | *c*, *c* | 5<br>5 | 8<br>6 | 6<br>8 |
| 4 | 2 | −1 | *c* | 1 | 4 | 6 |
| 4 | −2 | 1 | — | $n$ | $2n$ | $2n$ |
| 4 | −2 | −1 | *c* | $3n$ | $4n$ | $2n$ |
| 4 | 3 | −1 | *c* | $n$ | $2n$ | $4n$ |
| 4 | −3 | −1 | *a*, *c* | 7 | 8 | 2 |
| 4 | −3 | 2 | — | $n$<br>5 | $2n$<br>6 | $2n$<br>2 |
| 4 | 3 | −3 | *b* | $3n$<br>6 | $2n$<br>1 | $4n$<br>7 |
| 5 | 1 | −1 | *b* | $n$<br>3<br>4 | $2n$<br>2<br>1 | $3n$<br>7<br>9 |
| 5 | −1 | −1 | — | $n$<br>$n$ | $n$<br>$2n$ | $2n$<br>$n$ |
| 5 | 2 | −2 | *b* | 4 | 3 | 7 |
| 5 | −2 | −2 | — | $2n$<br>$2n$ | $3n$<br>$n$ | $n$<br>$3n$ |
| 5 | 3 | −2 | — | $n$<br>$n$<br>5 | $n$<br>$3n$<br>1 | $2n$<br>$4n$<br>8 |
| 5 | −3 | −2 | *a* | 5<br>7 | 3<br>9 | 7<br>1 |
| 5 | 3 | −3 | *b* | $3n$<br>3 | $n$<br>7 | $4n$<br>8 |
| 6 | 1 | −1 | *b* | 2<br>2 | 1<br>5 | 5<br>7 |
| 6 | −2 | −1 | — | $n$<br>3 | $n$<br>5 | $2n$<br>2 |
| 6 | 3 | −1 | — | $n$<br>1 | $n$<br>5 | $3n$<br>9 |
| 6 | 3 | −2 | — | $n$<br>5 | $2n$<br>2 | $3n$<br>9 |

As $k_c$ usually occurs in two or more places among $q_i - M_j A$, it is possible to find $k_c$. Among the numbers $q_i - M_j A$ for $i = 2$, 4 or 5 (in the given example), one then looks for $4k_c$, $9k_c$, etc., and possibly also for $k_c/4$, $9k_c/4$, etc. or $k_c/9$, $4k_c/9$, etc. In the case where all the first reflexions have different indices, $l$, one of the numbers $q_1 - M_j A$ will equal $k_c$. One then tests these numbers in turn in the same way as above.

If $C$ is given, $A$ can be found in an analogous way. A larger number of lines ought to be considered in this case.

### 1·3. Formation of the expressions $\Sigma k_i q_i = 0$

If the smallest $q$ values observed are

$$q_1 < q_2 < q_3 < q_4 < q_5 \cdots < q_n,$$

one forms among these all the sums $q_i + q_j \leqq R$ ($R$, for example, $= q_{10}$, $i \leqq j$), according to the scheme given below:

| | $q_1$ | $q_2$ | $q_3$ | $q_4$ | $q_5$ | $q_6$ |
|---|---|---|---|---|---|---|
| $q_1$ | $2q_1$ (4) | | | $q_4 - q_1$(4) | $q_5 - q_1$(3) | $q_6 - q_1$ |
| $q_2$ | $q_1 + q_2$(3) | $2q_2$ | | | $q_5 - q_2$ | $q_6 - q_2$ |
| $q_3$ | $q_1 + q_3$(1) | $q_2 + q_3$ | $2q_3$ | | $q_5 - q_3$ | $q_6 - q_3$ |
| $q_4$ | $q_1 + q_4$ | $q_2 + q_4$(2) | $q_3 + q_4$ | $2q_4$ | | |
| $q_5$ | $q_1 + q_5$(2) | $q_2 + q_5$ | $q_3 + q_5$ | $q_4 + q_5$ | $2q_5$ | |
| $q_6$(1) | $q_1 + q_6$ | $q_2 + q_6$ | $q_3 + q_6$ | | | |
| $q_7$ | $q_1 + q_7$ | $q_2 + q_7$ | | | | |

In this scheme one looks for sums or single $q$ values which are equal within narrow limits of error. (One notices that values of approximately the same magnitude occur near lines which are parallel to the dotted line in the scheme.) The limits of error are discussed in § 3; in all cases hitherto treated we have put $q_i + q_j = q_s$ if $q_i + q_j = q_s + \Delta$, where $|\Delta| \leqq 0{\cdot}0005$. If in this way one has found that the numbers indicated by (1) in the scheme are equal, one gets the equation $q_1 + q_3 = q_6$. In the same way the numbers indicated by (2) give $q_1 + q_5 = q_2 + q_4$. Consequently, one obtains equations of the types $q_i + q_j = q_s$ and $q_i + q_j = q_s + q_r$. From these equations one obtains separate expressions in $l^2$ and $M$ from which the indices can be calculated. It is convenient first to carry out eliminations within the system so that equations of the types $\sum^3 k_i q_i = 0$ (one $k_i > 1$) or $k_i q_i = k_j q_j$ are obtained.

If the sums do not give a sufficient number of equations, one can also form differences $q_i - q_j \geqq 2q_1$. It is of no use to look for equalities among the differences only. They repeat relations obtained earlier from the sums; for if $q_i - q_j = q_s - q_r$, then $q_i + q_r = q_s + q_j$. Equalities between differences and sums, however, give the desired equations. The equalities (3) in the scheme give $q_5 = 2q_1 + q_2$, whereas (4) give $q_4 = 3q_1$. In forming the equations one excludes equations which are not independent. It is easily seen that one of the equations (2), (3), (4) is superfluous.

Another way of directly obtaining equations of the types $\sum^3 k_i q_i = 0$ (one $k_i > 1$) and $k_i q_i = k_j q_j$ without eliminations is to form sums (and differences if necessary) of the numbers $q_1$, $2q_1$, $q_2$, $2q_2$, $q_3$, $2q_3$ and so on. These numbers are arranged in increasing order and the summations are carried out in the same way as in the scheme above. (An example of this procedure is given in § 1·5, example 2.)

### 1·4. Performance of the indexing

It is supposed that the $q$ values of all lines with small angles of deviation have been determined with the greatest possible accuracy (see § 3). If one has found that the system is non-cubic, equations are formed according to § 1·3, after which solutions in $M$ and $l^2$ are determined as in § 1·1. If only $A$ or $mA$ is obtained in this way, $C$ is determined according to § 1·2. The method of § 1·2 can also be used for lines of higher angles as a check on the values of $A$ and $C$ already obtained. If $A : C$ is equal or nearly equal to a quotient between small integers, certain equations cannot be treated by representation by number pairs. In this case one has to look for solutions of each equation separately; this leads to several alternatives.

Finally, one can try to determine one constant by the method used for the orthorhombic case (see § 2).

### 1·5. Applications

The above method of indexing powder photographs of tetragonal and hexagonal crystals has been successfully tried on several cases where the author did not know anything about symmetry or dimensions beforehand. One such case was the second of the two examples given below, both of which have been taken from investigations by Kiessling (1947).

*Example* 1. $W_2B$; Cr $K\alpha_1$ *radiation*

The nine lowest $\sin^2\theta$ values are:

$$q_1 = 0{\cdot}0847, \quad q_4 = 0{\cdot}2698, \quad q_7 = 0{\cdot}4025,$$
$$q_2 = 0{\cdot}1694, \quad q_5 = 0{\cdot}3179, \quad q_8 = 0{\cdot}4229,$$
$$q_3 = 0{\cdot}2334, \quad q_6 = 0{\cdot}3384, \quad q_9 = 0{\cdot}5724.$$

Sums $q_i + q_j \leqq q_9$ are formed according to § 1·3:

| | | $q_1$ | $q_2$ | $q_3$ | $q_4$ |
|---|---|---|---|---|---|
| $q_1$ | 0·0847 | 0·1694 (1) | | | |
| $q_2$ | 0·1694 (1) | 0·2541 | 0·3388 (3) | | |
| $q_3$ | 0·2334 | 0·3181 (2) | 0·4028 | 0·4668 | |
| $q_4$ | 0·2698 | 0·3545 | 0·4392 | 0·5032 | 0·5396 |
| $q_5$ | 0·3179 (2) | 0·4026 (4) | 0·4873 | 0·5513 | |
| $q_6$ | 0·3384 (3) | 0·4231 (5) | 0·5078 | 0·5718 | |
| $q_7$ | 0·4025 (4) | 0·4872 | 0·5719 (6) | | |
| $q_8$ | 0·4229 (5) | 0·5076 | | | |
| $q_9$ | 0·5724 (6) | | | | |

The following independent equations are obtained:

$$(1)\ 2q_1 = q_2, \quad (3)\ 2q_2 = q_6, \quad (5)\ q_1 + q_6 = q_8,$$
$$(2)\ q_1 + q_3 = q_5, \quad (4)\ q_1 + q_5 = q_7, \quad (6)\ q_2 + q_7 = q_9,$$

which give

$$(7)\ q_6 = 4q_1, \qquad (9)\ q_8 = 5q_1,$$
$$(8)\ q_7 = q_3 + 2q_1, \qquad (10)\ q_9 = q_3 + 4q_1.$$

From (1), (2), (7), (8), (9) and (10) one obtains ($q_2$), ($q_5$), ($q_6$), ($q_7$), ($q_8$) and ($q_9$) directly expressed in $M_1$, $l_1^2$, $M_3$ and $l_3^2$.

The equations (1), (3) and (9) each show that the system is tetragonal, and that, among others, $l_1 = 0$. Hence, $A = 0{\cdot}0847/M_1$.

$M_3 < 3M_1$ because $q_3 < 3q_1$. Moreover, $M_3 \neq 2M_1$, otherwise equation (2) gives $M_5 = 3M_1$ which is impossible in the tetragonal system. In the same way one obtains $M_3 \neq M_1$, $M_1/2$, and $5M_1/2$. We first try $M_1 \leqq 2$ according to the method in § 1·2. In this case the above gives $M_3 = 0$ and $Cl_3^2 = 0{\cdot}2334$. It is then only necessary to form $q_4 - AM_j$ as the rest of the lines are already expressed in $M_1$ and $l_3^2$.

For $M_1 = 1$, $A_1 = 0{\cdot}0847$:

$$q_4 = 0{\cdot}2698, \quad q_4 - A_1 = 0{\cdot}1851, \quad q_4 - 2A_1 = 0{\cdot}1005.$$

Neither of these numbers is related in a simple way to $Cl_3^2$.

For $M_1 = 2$, $A_1 = 2A_2$:

$$q_4 - A_2 = 0{\cdot}2275, \quad q_4 - 5A_2 = 0{\cdot}0581 = Cl_3^2/4,$$

whence $M_4 = 5$ and $l_3^2 = 4l_4^2$. For $l_4 = 1$, which gives $l_3 = 2$, all lines will be indexed according to equations (1), (2), (7), (8), (9) and (10) in the following way:

$$(q_1) = (2, 0), \quad (q_4) = (5, 1), \quad (q_7) = (4, 4),$$
$$(q_2) = (4, 0), \quad (q_5) = (2, 4), \quad (q_8) = (10, 0),$$
$$(q_3) = (0, 4), \quad (q_6) = (8, 0), \quad (q_9) = (8, 4).$$

*Example* 2. *δ-phase in the system* Mo-B; Cr $K\alpha_1$ *radiation*

The first eleven $\sin^2\theta$ values are:

$$q_1 = 0{\cdot}0732, \quad q_4 = 0{\cdot}2502, \quad q_7 = 0{\cdot}4361, \quad q_{10} = 0{\cdot}6165,$$
$$q_2 = 0{\cdot}1406, \quad q_5 = 0{\cdot}2910, \quad q_8 = 0{\cdot}5050, \quad q_{11} = 0{\cdot}6561,$$
$$q_3 = 0{\cdot}1771, \quad q_6 = 0{\cdot}3595, \quad q_9 = 0{\cdot}5441.$$

Here the sums $< q_8$ of the numbers $q_1$, $q_2$, $2q_1$, $q_3$, $q_4$, $2q_2$, $q_5$, $2q_3$ and $q_6$ are formed:

| | $q_1$ | $q_2$ | $2q_1$ | $q_3$ | $q_4$ |
|---|---|---|---|---|---|
| $q_1$ 0·0732 | 0·1464 | | | | |
| $q_2$ 0·1406 | 0·2138 | 0·2812 | | | |
| $2q_1$ 0·1464 | 0·2196 | 0·2870 | 0·2928 | | |
| $q_3$ 0·1771 | 0·2503 (1) | 0·3177 | 0·3235 | 0·3542 | |
| $q_4$ 0·2502 (1) | 0·3234 | 0·3908 | 0·3966 | 0·4273 | 0·5004 (3) |
| $2q_2$ 0·2812 | 0·3544 (2) | 0·4218 | 0·4276 | 0·4583 | |
| $q_5$ 0·2910 | 0·3642 | 0·4316 | 0·4374 | 0·4681 | |
| $2q_3$ 0·3542 (2) | 0·4271 | 0·4948 | 0·5006 | | |
| $q_6$ 0·3595 | 0·4327 | 0·5001 (3) | 0·5059 | | |

The following independent equations are obtained:

$$(1)\ q_4 - q_3 - q_1 = 0, \quad (2)\ 2q_3 - 2q_2 - q_1 = 0,$$
$$(3)\ 2q_4 - q_6 - q_2 = 0.$$

From Table 2 we find that these equations have the following solutions in $l$ in common:

(*a*) $l_1 = l_2 = l_3 = l_4 = l_6 = 0$, which requires

$$q_1 : q_2 : q_3 : q_4 : q_6 = M_1 : M_2 : M_3 : M_4 : M_6.$$

No acceptable ratios of this kind exist, whence this solution is excluded.

(*b*) $l_1 = 0$, $l_2 = l_3 = l_4 = l_6$, whence $AM_1 = 0{\cdot}0732$. According to (2) $M_1$ must be divisible by 2. A study of possible $M_2$ values in (1), (2) and (3) excludes $M_1 = 2$. Hence, $M_1$ must be $= 4, 8, 10$, etc. Though the low-angle lines can thus be indexed, contradictions occur for lines with larger angles. Hence, the only remaining possibility will be:

(*c*) $l_1 = 4$, $l_2 = 1$, $l_3 = 3$, $l_4 = 5$, $l_6 = 7$. Here $M_1$ can be $= 0, 4, 8, 10$, etc. If $M_1 = 0$, then $M_2 = M_3 = M_4 = M_6$. Further $q_1 = 16C = (q_6 - q_2)/3 = 0{\cdot}0729_6$, $q_{11}/9 = 0{\cdot}0729$. We use the accurate value $C = q_{11}/144$ and calculate $q_i - Cl_j^2$ for $i = 6$, 7, 8, etc. ($q_5 = 64C$). In this way the system is found to be tetragonal and the indexing of all lines is possible. The value of $A$ is found to be 0·1360. A great number of reflexions are missing, but practically all of them correspond to the absences required by the space group $D_{4h}^{19}$–$I4/amd$. The large percentage of absences and the high axial ratio ($c/a = 5{\cdot}465$) would have rendered an indexing of this photograph by means of graphical methods very difficult.

## 2. ORTHORHOMBIC SYSTEM

### 2·1. General relations

The indexing of powder photographs of orthorhombic crystals requires a great number of $\sin^2\theta$ values.

The quadratic form of the orthorhombic system is

$$q_i = A_1 h_{1i}^2 + A_2 h_{2i}^2 + A_3 h_{3i}^2, \quad \text{where} \quad q_i = \sin^2\theta_i.$$

If two of the constants ($A_1$ and $A_2$) are known, the third constant ($A_3$) can be determined immediately according to the method given in § 1·2.

If only one of the constants (e.g. $A_1$) is known, the problem is brought back to the indexing of

$$r_i = A_2 h_{2i}^2 + A_3 h_{3i}^2.$$

This indexing is carried out in the following way.

If
$$q_{i_1} = A_1 + A_2 h_{2i}^2 + A_3 h_{3i}^2$$
$$q_{i_2} = A_1 4 + A_2 h_{2i}^2 + A_3 h_{3i}^2$$
$$\cdots\cdots\cdots\cdots\cdots\cdots$$
$$q_{i_n} = A_1 n^2 + A_2 h_{2i}^2 + A_3 h_{3i}^2,$$

then

$$q_{i_1} - A_1 = q_{i_2} - 4A_1 = \ldots = q_{i_n} - A_1 n^2 = A_2 h_{2i}^2 + A_3 h_{3i}^2.$$

Consequently, one forms all numbers of the type $q_i - A_1 h^2 > 0$ for a great number of $q$ values. Among the numbers $q_i - A_1 h^2 > 0$, where $h$ also can equal 0, all numbers occurring twice or several times are picked out. These numbers are denoted by $r_1$, $r_2$, $r_3$, etc. Most of the numbers $r_i$ are usually of the form $A_2 h_{2i}^2 + A_3 h_{3i}^2$. Index combinations which are not to be found among the given $q$ values may occur here.

If $r_i = A_2 h_{2i}^2 + A_3 h_{3i}^2$, then $r_i$ is represented by the number pair $(r_i) = (h_{2i}^2, h_{3i}^2)$. Under the same assumptions as for the tetragonal and hexagonal systems we obtain that if $r_{i_1} + r_{i_2} = r_s$, then

$$(h_{2i_1}^2, h_{3i_1}^2) + (h_{2i_2}^2, h_{3i_2}^2) = (h_{2s}^2, h_{3s}^2).$$

Hence (we assume $h < 10$):

(*a*) If $h_{2s}^2$ and $h_{3s}^2 \neq 25$, then one $(r_i)$ is equal to $(h_{2s}^2, 0)$ and the other to $(0, h_{3s}^2)$.

(*b*) If $h_{2s}^2 = 25$ and $h_{3s}^2 \neq 25$, then one $(r_i)$ is equal to $(h_{2i}^2, 0)$, where $h_{2i}^2 = 9$, 16 or 25.

(*c*) If $h_{2s}^2 = h_{3s}^2 = 25$, then one $(r_i)$ is equal to (25, 0), (16, 9) or (16, 16).

(If in the last case $(r_{i_1}) = (16, 16)$, then $r_{i_1} : r_s = 16 : 25$.) We thus determine $A_2$ and $A_3$ with the aid of equations of the type $r_{i_1} + r_{i_2} = r_s$. After finding $A_2$, $A_3$ is determined according to § 1·2. In doing this one must (as when treating the equation $r_{i_1} + r_{i_2} = r_s$) pay regard to the fact that not all $r$'s are always of the form

$$r = A_2 h_2^2 + A_3 h_3^2.$$

The determination of one or several of the constants $A$ *ab initio* is carried out in the following way:

If $q_1 < q_2 < q_3 < \dots < q_n$ (say that $n$ is about 40) all expressions $q_i + q_j = q_s$ ($s \leq n$ and $i$, say, $\leq 10$) are formed according to § 1·3. It is extremely probable that $q_i$'s of the type $q = Ah^2$ will occur in a great number of these equations. In all cases hitherto treated the $q_i$ value which has been most frequent in such equations has been of this type. The expressions $q_i + q_j = q_s$ are formed using a narrow margin for the errors of measurement.

One also forms differences of the type $0 < (q_s - q_j) < q_1$. If $A < q_1$, numbers of the type $A_1(h_{1s}^2 - h_{1j}^2)$, $A_2(h_{2s}^2 - h_{2j}^2)$, $A_3(h_{3s}^2 - h_{3j}^2)$ will be found among the most frequent differences. The formation of differences $> q_1$ is generally unnecessary, as also the formation of differences between all given $q$ values. It is convenient to plot the differences in a diagram (see the example below).

If $q_i^0$ is one of the numbers which is most frequent as term $q_i$ or $q_j$ in the expressions $q_i + q_j = q_s$, one tests if $q_i^0(n^2 - l^2)/m^2$ (where $m$, $n$ and $l$ are integers) is represented among the most frequent differences. If this is the case, one puts $q_i^0/m^2 = A_1$. With the value of $A_1$ thus obtained one tries to bring back the problem to the indexing of $A_2 h_{2i}^2 + A_3 h_{3i}^2$ in the manner given before. If both $A_1$ and $A_2$ are obtained in this way, $A_3$ is determined according to § 1·2.

If it is impossible to find any relation among the most frequent sums and differences one tests $A_1 = q_i^0$, $A_1 = q_i^0/4$, $A_1 = q_i^0/9$ and so on.

### 2·2. Application

Several powder photographs of orthorhombic crystals, which were unknown to the author, have been indexed in this way. One typical example is given here.

*Example* 3. $KNO_3$, Cr $K\alpha_1$ *radiation*

The forty lowest observed $\sin^2\theta$ values are:

| | | | |
|---|---|---|---|
| $q_1 = 0·0923$, | $q_{11} = 0·2264$, | $q_{21} = 0·3462$, | $q_{31} = 0·4663$, |
| $q_2 = 0·0943$, | $q_{12} = 0·2339$, | $q_{22} = 0·3481$, | $q_{32} = 0·4963$, |
| $q_3 = 0·1271$, | $q_{13} = 0·2411$, | $q_{23} = 0·3513$, | $q_{33} = 0·5239$, |
| $q_4 = 0·1392$, | $q_{14} = 0·2496$, | $q_{24} = 0·3689$, | $q_{34} = 0·5427$, |
| $q_5 = 0·1427$, | $q_{15} = 0·2678$, | $q_{25} = 0·3766$, | $q_{35} = 0·5551$, |
| $q_6 = 0·1720$, | $q_{16} = 0·2731$, | $q_{26} = 0·4177$, | $q_{36} = 0·5624$, |
| $q_7 = 0·1789$, | $q_{17} = 0·2818$, | $q_{27} = 0·4223$, | $q_{37} = 0·5693$, |
| $q_8 = 0·1853$, | $q_{18} = 0·3060$, | $q_{28} = 0·4287$, | $q_{38} = 0·5748$, |
| $q_9 = 0·1877$, | $q_{19} = 0·3122$, | $q_{29} = 0·4500$, | $q_{39} = 0·6151$, |
| $q_{10} = 0·1898$, | $q_{20} = 0·3263$, | $q_{30} = 0·4600$, | $q_{40} = 0·6699$. |

We form all expressions of the form $q_i + q_j = q_s$ for $i \leq 10$, $s \leq 40$:

$$\begin{array}{llll}
q_1+q_{10}=q_{17}, & q_2+q_{17}=q_{25}, & q_4+q_5=q_{17}, & q_7+q_{25}=q_{35}, \\
q_1+q_{12}=q_{20}, & q_3+q_7=q_{18}, & q_5+q_{11}=q_{24}, & q_8+q_{25}=q_{36}, \\
q_1+q_{29}=q_{34}, & q_3+q_8=q_{19}, & q_5+q_{12}=q_{25}, & q_9+q_{13}=q_{28}, \\
q_2+q_4=q_{12}, & q_3+q_{14}=q_{25}, & q_6+q_7=q_{23}, & q_{10}+q_{18}=q_{32}. \\
q_2+q_7=q_{16}, & q_3+q_{24}=q_{32}, & q_7+q_{10}=q_{24}, & \\
q_2+q_9=q_{17}, & q_3+q_{34}=q_{40}, & q_7+q_{14}=q_{28}, &
\end{array}$$

The frequencies of $q_1, q_2, \dots q_{10}$, in these expressions are

$$q_1(3),\quad q_2(4),\quad q_3(5),\quad q_4(2),\quad q_5(3),\quad q_6(1),$$
$$q_7(6),\quad q_8(2),\quad q_9(2),\quad q_{10}(3).$$

The numbers $q_7(6)$, $q_3(5)$ and $q_2(4)$ are evidently of special interest.

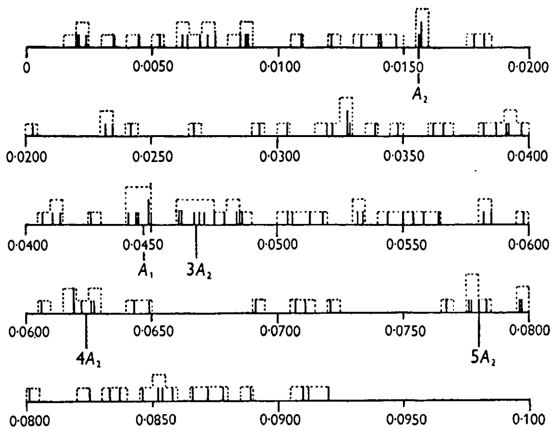


Fig. 1. Numerical interpretation of orthorhombic powder photograph.

In Fig. 1 the occurrence of values $q_s - q_j$ ($< q_1$) for $s \leq 20$ is indicated by vertical lines on the abscissa. If two values coincide, the line is given double the height. The distribution of these values is further shown by the areas enclosed by dotted lines, the height of which is proportional to the number of differences $q_s - q_j$ falling within an interval of $5 \times 10^{-4}$ on the abscissa.

From the diagram we see that no less than five differences are situated in the immediate vicinity of $q_7/4 = 0·0447$. The numbers $q_2$ and $q_3$ do not show any simple relations with the differences. We put $q_7/4 = A_1$ and form $q_j - A_1 h^2 > 0$ for all given $q$ values. (If no result had been obtained in this way, we would have tested $A_1 = q_7/16$* or possibly $A_1 = q_7/36$.)

From the numbers $q_j - A_1 h^2 > 0$ (where $h$ also can be zero) we obtain the following $r$ values (the numerical

* When testing $A_1 = q_7/16$ it is necessary to form only the new numbers $q_j - A_1$, $q_j - 9A_1$, $q_j - 25A_1$, etc. The rest of the numbers have already been formed for $A_1 = q_7/4$.

values given being means of the different numbers giving practically the same $r$ value):

$$
\begin{aligned}
r_1 &= 0{\cdot}0475 = q_1 - A_1 = q_{11} - 4A_1 = q_{29} - 9A_1,\\
r_2 &= 0{\cdot}0942 = q_2 = q_4 - A_1 = q_{16} - 4A_1 = q_{32} - 9A_1{}^*,\\
r_3 &= 0{\cdot}1272 = q_3 = q_6 - A_1 = q_{18} - 4A_1,\\
r_4 &= 0{\cdot}1404 = q_8 - A_1 = q_{34} - 9A_1,\\
r_5 &= 0{\cdot}1428 = q_5 = q_9 - A_1,\\
r_6 &= 0{\cdot}1670 = q_{21} - 4A_1 = q_{37} - 9A_1,\\
r_7 &= 0{\cdot}1722 = q_6 = q_{23} - 4A_1 = q_{38} - 9A_1,\\
r_8 &= 0{\cdot}1895 = q_{10} = q_{12} - A_1,\\
r_9 &= 0{\cdot}2497 = q_{14} = q_{28} - 4A_1,\\
r_{10} &= 0{\cdot}2676 = q_{15} = q_{19} - A_1 = q_{40} - 9A_1,\\
r_{11} &= 0{\cdot}2815 = q_{17} = q_{20} - A_1 = q_{30} - 4A_1,\\
r_{12} &= 0{\cdot}3063 = q_{18} = q_{23} - A_1,\\
r_{13} &= 0{\cdot}3764 = q_{25} = q_{35} - 4A_1,\\
r_{14} &= 0{\cdot}3838 = q_{28} - A_1 = q_{36} - 4A_1,\\
r_{15} &= 0{\cdot}4220 = q_{27} = q_{31} - A_1,\\
r_{16} &= 0{\cdot}5242 = q_{33} = q_{37} - A_1.
\end{aligned}
$$

All equations of the type $r_{i_1} + r_{i_2} = r_s$ are formed ($\Delta \leqq 0{\cdot}0005$):

(1) $r_3 + r_4 = r_{10}$, (3) $r_4 + r_{11} = r_{15}$, (5) $r_4 + r_{14} = r_{16}$,

(2) $r_3 + r_9 = r_{13}$, (4) $r_7 + r_9 = r_{15}$.

We consider the equations (1) and (2):

Both $(r_{10})$ and $(r_{13})$ cannot be (25, 25). Then according to (1) and (2) one of the number pairs $(r_3)$, $(r_4)$ or $(r_9)$ must be equal to $(h_{2i}^2, 0)$ (or to $(0, h_{3i}^2)$, which is the same). Further, $r_4 : r_9 = 9 : 16$ and, consequently, $16h_{24}^2 = 9h_{29}^2$ and $16h_{34}^2 = 9h_{39}^2$. We assume $(r_4) = (9, 0)$ requiring $(r_9) = (16, 0)$, whence, according to (1) and (2), $(r_3) = (0, h_{33}^2)$. Then

$$A_2 = r_9/16 = 0{\cdot}0156 \quad \text{and} \quad A_3 = r_3/h_{33}^2 = 0{\cdot}1272/h_{33}^2.$$

According to § 1·2 we form $r_i - A_2h^2 > 0$ for $i = 1, 2, 5, 6, 7$ and 8, from which $A_3 = r_3/4 = 0{\cdot}0318$ and $(r_1) = (1, 1)$, $(r_2) = (4, 1)$, $(r_3) = (0, 4)$, $(r_5) = (1, 4)$, $(r_7) = (9, 1)$ and $(r_8) = (4, 4)$. It is not possible to obtain the indices of $r_6$ in this connexion.

From (1), (2), (4) and (3) we now obtain directly

$$(r_{10}) = (9, 4), \; (r_{13}) = (16, 4), \; (r_{15}) = (25, 1)$$

and $\qquad (r_{11}) = (16, 1)$.

Equation (5), on the other hand, leads to a paradox. The constants obtained do not permit the indexing of $r_{12}$ and $r_{14}$, but it is too much to assume that all $r_i$ are of the form $A_2h_{2i}^2 + A_3h_{3i}^2$.

We further find that $(r_{16}) = (1, 16)$.

---

* The fact that $r_2$ can be expressed in four different ways in $A_1$ and $q$ supports the assumption that $A_1 = q_7/4$.

With the aid of the indices of $r_i$ (except $r_6$, $r_{12}$ and $r_{14}$) and the connexions between $q_j$ and $r_i$ (see above) we obtain *directly* the indices of all lines except $q_7$, $q_{13}$, $q_{21}$, $q_{22}$, $q_{24}$, $q_{26}$, $q_{36}$ and $q_{39}$. It is, however, possible to index these lines with the constants now obtained. In this way the whole photograph has been indexed.

*Further remarks.* Fig. 1 shows accumulations of numbers round the values $A_2 = 0{\cdot}0156$, $(4-1)A_2 = 0{\cdot}0468$, $4A_2 = 0{\cdot}0624$ and $(9-4)A_2 = 0{\cdot}0780$. Moreover, number $q_3$, which occurs in five expressions of the type $q_i + q_j = q_s$, is equal to $4A_3$. ($q_2$, which occurs four times in the corresponding expression, is equal to $4A_2 + A_3$.)

A calculation of $A_3$ according to § 1·2 and with the assumptions $A_1 = q_7/n^2$ and $A_2 = q_3/m^2$, would have led to a result more rapidly than the method described above, where $q_i - A_1h^2$ was formed. One would then have to test the alternatives $A_1 = q_7/16$, $A_2 = q_3/16$ and $A_1 = q_7/16$, $A_2 = q_3/9$. The first alternative makes possible the indexing of all lines with the indices $(2h_{1i}, 2h_{2i}, h_{3i})$ which gives $A_1 = q_7/4$ and $A_2 = q_3/4$.

## 3. ACCURACY OF MEASUREMENTS

An essential condition for the success of the indexing method here described is a high accuracy of the observed $q$ values. If the $q$'s or sums of $q$'s which are to be equated are not sufficiently well known, the risk of obtaining 'false equations' is obvious, especially if the cell dimensions are large. Only a single false equation has occurred in all the cases investigated by the author, mainly owing to the high accuracy of the experimental material. False equations will probably be easy to rule out by internal inconsistency.

The author used exclusively focusing cameras of the Seemann-Bohlin type, modified by Phragmén (Westgren, 1931) and later by Hägg. Some geometrical constants of these cameras are given by Hägg & Regnström (1944). The measurement of the film was carried out according to the method described by Hägg (1947), in which an automatic correction for film shrinkage is obtained. With suitable preparations the error of a single measurement will never exceed $\pm 0{\cdot}1$ mm. and in most cases will not exceed $\pm 0{\cdot}07$ mm. The effect of an error of 0·1 mm. on the value of $q$ ($= \sin^2\theta$) in different ranges of the three cameras (A, B and C) used is given in Table 3.

Table 3. *Error in $q$ ($= \sin^2\theta$) caused by an error in line position of* 0·1 *mm.*

| Camera | $q$ | Error in $q$ |
|---|---|---|
| A | 0·065–0·240 | 0·0001–0·0002 |
| B | 0·180–0·615 | 0·0003–0·0004 |
| C | 0·525–0·790 | 0·0005–0·0004 |
| | 0·790–0·900 | 0·0004–0·0003 |
| | 0·900–0·955 | 0·0003–0·0002 |
| | 0·955–0·980 | 0·0002–0·0001 |

As a consequence one can consider the maximum error in $q$ to be $\pm 0{\cdot}0005$. It is highly probable that no real equations in $q$ would be missed by rejecting coincidences between $q$-sums or $q$-differences which differ by an amount exceeding 0·0004. In the examples given above, however, the value 0·0005 was chosen.

In order to get the above accuracy with a camera of the Debye-Scherrer type the camera diameter must be large. With a diameter of 19 cm. an error of 0·1 mm. in line position will cause an error in $q$ of 0·0005 for lines with a mean deviation ($2\theta$) of 90°.

I wish to thank Prof. G. Hägg for his constant interest and help during the preparation of this paper.

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*Acta Cryst.* (1948). **1**, 207

# Multiple Guinier Cameras

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(*Received* 12 *March* 1948 *and in revised form* 2 *June* 1948)

The novel type of Guinier camera described in this paper is characterized by a combination of several cameras in a compact unit using a single focusing monochromator and a single film, and by the disposition of the camera relative to the monochromator in such a manner that $\alpha$-doublet diffraction lines coincide for a $\theta$ value of, say, 15°. In this way an exceptionally high resolving power is obtained in a considerable range of glancing angles, centred about this value, which contains the most selective lines for analytical purposes. The line width in the respective cameras is discussed, and the conclusion is reached that in the significant region $\theta < 30°$ there is no appreciable difference between the outer and the middle cameras of the unit. With a view to comparison purposes, the line shift for the outer cameras is also calculated; it appears to be of little consequence. Finally, short descriptions of a twofold and of a fourfold camera are given.

## Introduction

In 1939 Guinier described a new type of focusing powder camera in which a convergent X-ray beam produced by a curved crystal monochromator passes through the specimen. Diffracted rays for any glancing angle $\theta$ converge to sharp diffraction lines on a film lying on the circular cylinder which contains the focal line and the sample (Fig. 1). As advantages of the new method compared with common powder diffraction technique, Guinier (1945, p. 147) has enumerated the low background intensity arising from the absence of white radiation, the good resolving power, and the large specimen volume, yielding smooth diffraction lines.

In our opinion, Guinier in this recapitulation (duly completed with the disadvantages: restricted $\theta$-range; rather difficult preparation of samples; exact focusing only in one plane) has by no means exhausted the merits of his achievement. In fact, after about a year of experience with Guinier cameras we think that they possess some unique features, to witness:

(*a*) The exceptionally high resolving power in the $\theta$-range for which the Guinier camera is suited, i.e. $\theta < 30°$. The resolving power in this range is essentially much better than with a Debye-Scherrer camera of the same dispersion for two reasons: (1) The focusing property eliminates to a large extent the influence of the thickness of the specimen. (2) Pairs of diffraction lines corresponding to both wave-lengths of the $\alpha$-doublet can be made to coincide for any desired value of $\theta$,

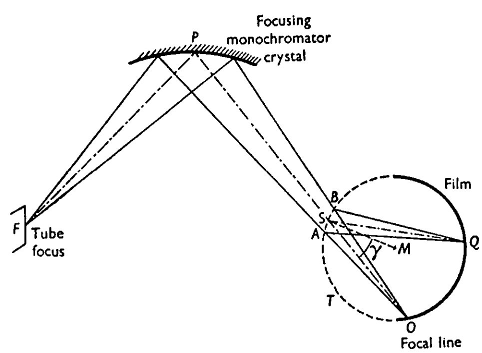


Fig. 1. Schematic plan of the Guinier camera. $F$, tube focus; $OQ$, film; $S$, specimen; $O$, focal line; $P$, focusing monochromator crystal.