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Abstract

A convenient and rapid slide-rule method for solving
electron diffraction patterns is described.
1. Introduction

With the rapid development and wide use of transmission electron microscopy in recent years and the necessity for indexing large numbers of diffraction patterns, a systematic, rapid and convenient method for indexing such patterns is extremely useful to the microscopist. This note describes a simple slide rule technique for this purpose.

2. Analysis of Diffraction Patterns

The electron diffraction pattern is a magnified image of a plane of the reciprocal lattice lying normal to the incident electron beam as shown in Fig. 1. It follows from this figure that the distance \( r \) from the origin of the diffraction pattern to a diffraction spot and the distance \( d^{-1} \) from the origin in reciprocal space to the corresponding reciprocal lattice point are related by the well known expression \( \lambda L = rd \) where \( L \) is the specimen to plate distance (and includes the magnification), \( \lambda \) is the wavelength and \( d \) the spacing of the reflecting planes \((hkl)\). The product \( \lambda L \) is known as the camera constant and is constant for a given photographic plate, thus

\[
\lambda L = r_1 d_1 = r_2 d_2 = r_n d_n
\]

therefore

\[
\frac{r_1}{r_2} = \frac{d_2}{d_1}, \quad \frac{r_1}{r_n} = \frac{d_n}{d_1}, \text{ etc.}
\]

Thus the ratios of the distances measured on the plate are equal to the ratios of the corresponding \( d \)-spacing for all crystals. The same result applies to measurements of Kikuchi line spacings.
3. Method of Indexing

In order to illustrate the technique, consider the case for cubic crystals. The \( d \)-spacings of planes \((hkl)\) are given by

\[
d_1 = \frac{a}{\sqrt{h_1^2 + k_1^2 + l_1^2}}
\]

Substituting in (1)

\[
\frac{r_1}{r_n} = \frac{d_n}{d_1} = \frac{(h_1^2 + k_1^2 + l_1^2)^{\frac{1}{2}}}{(h_n^2 + k_n^2 + l_n^2)^{\frac{1}{2}}} = \frac{(N_1)^{\frac{1}{2}}}{(N_n)^{\frac{1}{2}}}
\]

This shows that the interplanar spacings and the spot distances can be related without a knowledge of \( \lambda L \) or the lattice constant. An individual diffraction pattern can be indexed by obtaining the ratios of the \( r \) distances measured on the diffraction pattern and comparing them with the ratios for \((N)^{\frac{1}{2}}\). The latter ratios can be tabulated for convenient comparisons.

However, when these ratios are compiled into tabular form, it is necessary to first obtain the ratios of the \( r \) values from measurements and mathematical manipulation and then determine from the tables which planes correspond to this ratio. However, this part of the analysis can be shortened to give a more rapid answer and the necessity for tables can be eliminated, if a slide rule is used.

The standard slide rule is utilized such that numbers appearing on the A and B scales are the squares of the numbers appearing directly below them on the C and D scales. If the \( r \) distances of two diffraction spots are measured from an electron diffraction pattern and the ratio of these are obtained by division on the C and D scales, then two (or more) integral
numbers (corresponding to the sum of the squares of the indices of the
two diffracting planes) will be brought into coincidence on the A and B
scales. The ratio thus obtained on the C and D scales corresponds to the
ratio of the square roots of the two integral numbers brought into coincidence
on the A and B scales. Thus if it is known which integral numbers were
brought into coincidence and what planes are characterized by these numbers
(i.e., \( h_1^2 + k_1^2 + l_1^2 = N \)), indices can be quickly assigned to the two
diffraction spots which were measured on the diffraction pattern. (It
should be noted that a similar technique is often employed in indexing
rings obtained in x-ray powder patterns.) However, it would be much more
convenient, and there would be less chance of error if only the integral
numbers corresponding to the allowed reflections in the particular crystal
systems were present on the A and B scales. Going one step further, we
are not really interested in these numbers themselves, but only the planes
to which they correspond. Therefore, if a new A and B scale is used so that
the numbers are replaced by the indices of planes corresponding to the allowed
reflections, a slide rule is obtained which is capable of quickly giving the
indices of diffraction spots directly from the measured \( r \) distances on the
electron diffraction pattern.

A typical example of the use of the rule is illustrated in Fig. 2.
The distances \( r_1 \) and \( r_2 \) from the diffraction pattern in Fig. 2(a) (obtained
from a body centered cubic metal) are shown as they would appear on the
C and D scale in the front view of the rule (Fig. 2(b)) and the family of
planes corresponding to the spots (\( d \) and \( d' \)) on the diffraction pattern
are shown to be in coincidence in the back view of the slide rule (Fig. 2(c)).
Note that the face centered cubic allowed reflections and body-centered cubic
allowed reflections have been separated from each other on opposite sides of the slide to avoid possible intermixing of the two systems. It should be noted that the two planes, c and d, do not exactly line up. This is not an error or a shortcoming of the rule. It simply means that the pattern is tilted slightly away from the orientation as indexed, since it is possible for spots not actually lying exactly on the reflecting sphere to appear in the diffraction pattern. In order to assign specific indices to the various spots, it is necessary to check the indexing by measuring the angles between spots on different zones and confirming their indices from the relation

\[ \cos \phi = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)}} \]

In Fig. 2(a) the spots c and d have been indexed as: c = (321) and d = (121) with the angle \( \phi \) between them measured as 30°. This agrees with the calculated angle of 29° using the above formula.

Finally the foil orientation \([uvw]\) (i.e., the direction normal to the foil surface) is given by the cross product \([h_1 k_1 l_1] \times [h_2 k_2 l_2]\). For the diffraction pattern of Fig. 2(a) the result is \([121] \times [321] = [01\overline{2}]\). This cross product should be taken anticlockwise so that the sense is upward toward the observer. In this way comparison to a standard stereographic projection is facilitated for further crystallographic analysis. Furthermore, the correct sense of \([uvw]\) must be known if the sense of lattice displacements is to be determined.

More accurate determinations of the foil orientation are possible if the Kikuchi patterns are analysed.\(^{(1, 2)}\) If \(s_1\) and \(s_2\) are the distances between corresponding pairs of black and white Kikuchi lines on the plate, then the
ratios $S_1/S_2 = d_2/d_1$, etc., and the slide rule can be used to obtain the indices $h_1 k_1 l_1$, etc. from the $S$ ratios in exactly the same way as is used for the spot pattern.

Construction of the auxiliary $A$ and $B$ scales for the slide rule simply involves laying out on two cycle log paper the planes corresponding to $(h^2 + k^2 + l^2) = N$ and then photographically reducing it so that the length corresponds to the length of the $A-B$ scales (Fig. 2).

Similar scales can be used for other crystal systems - in fact rather than employ a number of slide rules, interchangeable scales can be used.

Acknowledgments

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References

Figure Captions

Fig. 1. Schematic representation of relationship of spots on a diffraction pattern and the spacing of corresponding planes in crystal.
\( \lambda L = r d \)

Fig. 2. Example of use of slide rule for indexing diffraction patterns.
(a) Diffraction pattern of body centered cubic crystal (niobium).
(b) Front view of slide rule showing \( r \) values of spots d and c on C and D scales.
(c) Back view of slide rule showing coincidence of planes \( (211) \) and \( (321) \) on auxiliary scales.
Fig. 1
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