Lawrence Berkeley National Laboratory

Recent Work

Title

SLIDE RULE METHOD FOR INDEXING ELECTRON DIFFRACTION PATTERNS

Permalink

<https://escholarship.org/uc/item/8vv033vc>

Authors

Roser, W.R.
Thomas, G.

Publication Date

1963-12-01

University of California
Ernest O. Lawrence
Radiation Laboratory

TWO-WEEK LOAN COPY

*This is a Library Circulating Copy
which may be borrowed for two weeks.
For a personal retention copy, call
Tech. Info. Division, Ext. 5545*

SLIDE RULE METHOD FOR INDEXING ELECTRON DIFFRACTION PATTERNS

Berkeley, California

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

UNIVERSITY OF CALIFORNIA
Lawrence Radiation Laboratory
Berkeley, California

AEC Contract No. W-7405-eng-48

SLIDE RULE METHOD FOR INDEXING ELECTRON DIFFRACTION PATTERNS

W. R. Roser and G. Thomas

December 1963

SLIDE RULE METHOD FOR INDEXING ELECTRON DIFFRACTION PATTERNS

W. R. Roser and G. Thomas

Inorganic Materials Research Division, Lawrence Radiation Laboratory
and Department of Mineral Technology, University of California
Berkeley, California

December, 1963

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), λ is the wavelength and d the spacing of the reflecting planes (hkl). The product λL 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

$$\frac{r_1}{r_2} = \frac{d_2}{d_1}, \quad \frac{r_1}{r_n} = \frac{d_n}{d_1}, \quad \text{etc.} \quad (1)$$

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

$$d_1 = a / \sqrt{h_1^2 + k_1^2 + l_1^2}$$

Substituting in (1)

$$\frac{r_1}{r_n} = \frac{d_n}{d_1} = \frac{(h_1^2 + k_1^2 + l_1^2)^{\frac{1}{2}}}{(h_n^2 + k_n^2 + l_n^2)^{\frac{1}{2}}} = \frac{(N_1)^{\frac{1}{2}}}{(N_2)^{\frac{1}{2}}}$$

This shows that the interplanar spacings and the spot distances can be related without a knowledge of λL 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 ϕ 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 $[121] \times [321] = [01\bar{2}]$. 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

We wish to thank the United States Atomic Energy Commission for financial support.

References

1. H. Wilman, Proc. Phys. Soc., 60, 341 (1948).
2. H. Wilman, Proc. Phys. Soc., 61, 416 (1948).

Figure Captions

Fig. 1. Schematic representation of relationship of spots on a diffraction pattern and the spacing of corresponding planes in crystal.

$$(\lambda L = rd)$$

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 $\sin^2 \theta$ 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.

MU-33305

Fig. 1

(a)

(b)

(c)

ZN-4107

Fig. 2

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

- A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or
- B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.