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A Geometrical Method for the Determination and Indexing of Electron Diffraction Patterns

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A geometrical method for the determination and indexing of electron diffraction patterns was developed by making use of descriptive geometry. This method is especially advantageous for noncubic structures. The general geometrical principles are presented, and a typical problem is solved in order to illustrate the procedures that can be followed to simplify the operations.

Introduction

The determination of allowed reflections and their indexing in electron diffraction patterns of materials having cubic structure rarely presents problems. One first calculates the geometrical structure factor for the cell in question: this gives the possible reflections for that type of lattice. In the case of electron diffraction, the Ewald sphere is considered as a plane due to its small curvature (large $1/\lambda$). Secondly, what is sought is the intersection of the Ewald plane, perpendicular to the incident electron beam—which is directed along the zone axis [HKL]—with the reciprocal lattice points (hkl). The satisfaction of the condition (1)

$$Hh + Kk + Ll = 0$$

permits one to determine the allowed reflections for a specific crystal. Points that almost meet this condition are also considered satisfactory because of the nonmonochromaticity of the incoming electron beam and of the disturbances in the lattice. Thirdly what is done is to draw the spots, bringing them to scale by inserting the camera constant and to compare the pattern determined thereby with the one obtained experimentally. One can then proceed to the indexing.

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In the other Bravais lattices the above procedure has to undergo some changes since planes and directions with equal indices lose their perpendicularity. The complications introduced can, however, be avoided by a graphical method presented herein.

Method

The method is a direct outgrowth of descriptive geometry (a branch of mathematics which has as its objectives the explanation of the methods of representation by drawing all geometrical magnitudes, and the solution of problems relating to these magnitudes in space [2, 3]). The "Mongean Method" is used here, for it is easier to operate on it, although the "Direct Method" could also be applied.

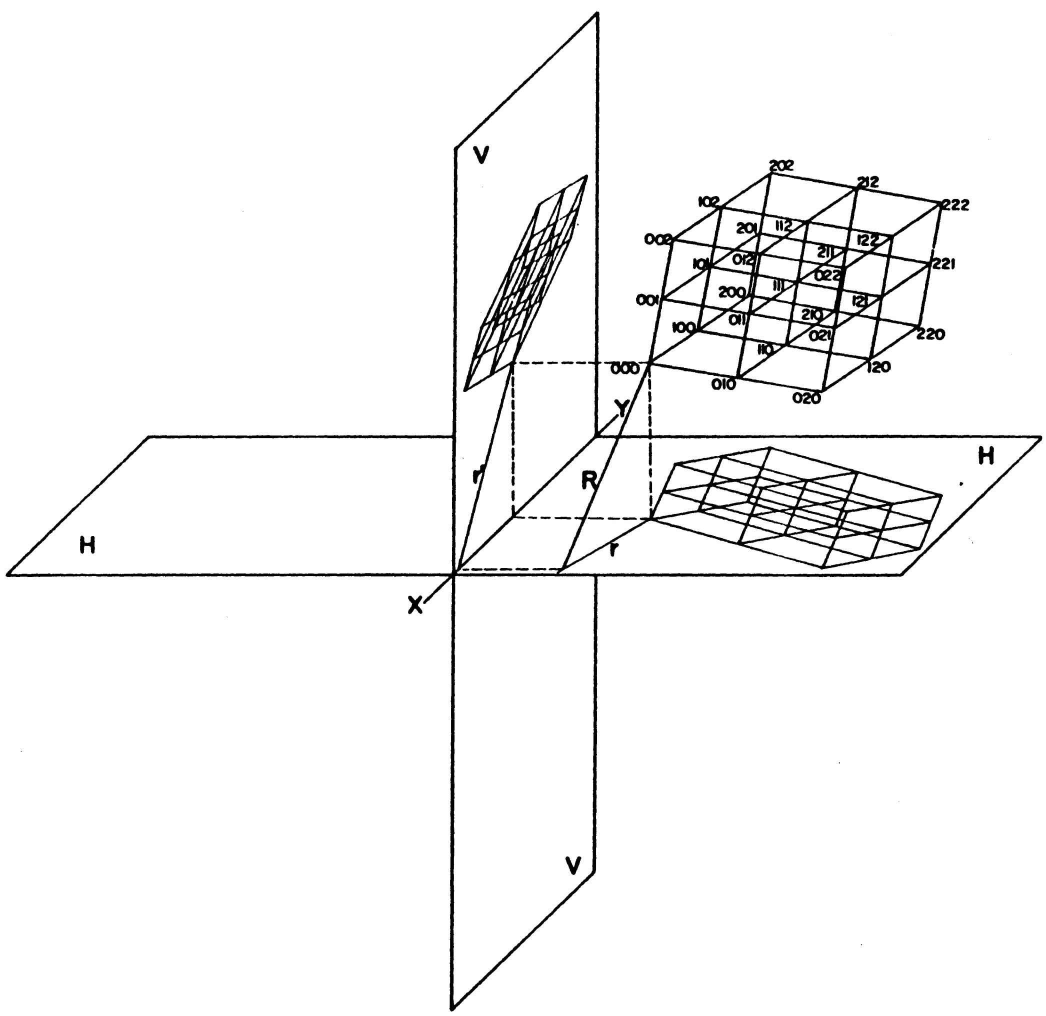

FIG. 1. Perspective view of a general cell.

The approach is straightforward. The problem could be proposed as the questions of what are the points of a reciprocal lattice which belong to a specific plane (the Ewald plane in question) and what is their distribution? The problem will be treated in two steps. Firstly, the general geometrical principles will be presented, and then a typical example will be introduced in order to demonstrate the method and what procedures can be followed to simplify the operations.

Figure 1 shows a perspective view of the most general unit cell (triclinic in reciprocal space) in a general orientation and a line (R) representing the direction of the incident electron beam. Orthographic projections of the unit cell and line (R) are made on the vertical plane of projection V and horizontal plane of projection H. The ground line is indexed (XY). After the plane V rotates about (XY), the two projections will be in the same plane and are shown in Fig. 2. One is now free to operate on this figure

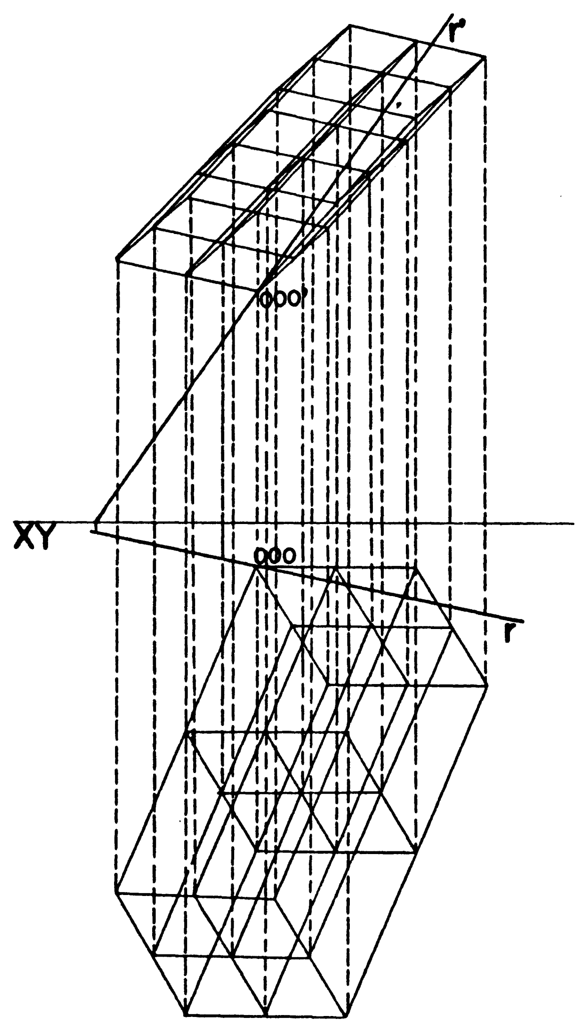

FIG. 2. Vertical and horizontal projections of a general cell.

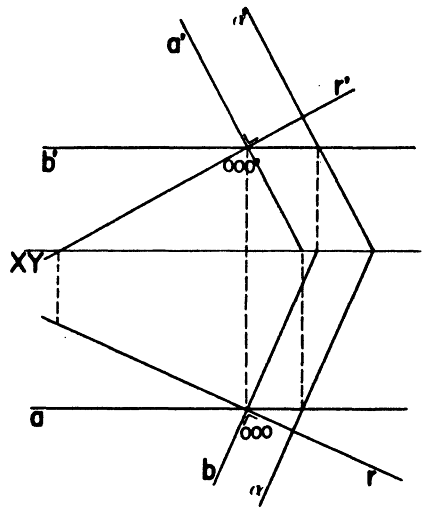

FIG. 3. Plane α passing through (000) and perpendicular to (R).

with the methods developed by descriptive geometry. This will be shown step-wise.

(a) Determination of a plane (α) passing through the reciprocal lattice origin and perpendicular to (R). This is shown in Fig. 3. First a horizontal (b) and a frontal line (a) are passed through (000) normal to (R). Then the traces (α) of the plane are determined.

(b) Determination whether a point belongs to the plane or not. This is done first in Fig. 4. The projection of a line (S) on one of the coordinate planes is traced so that it intersects the same projection of the point (mnp).

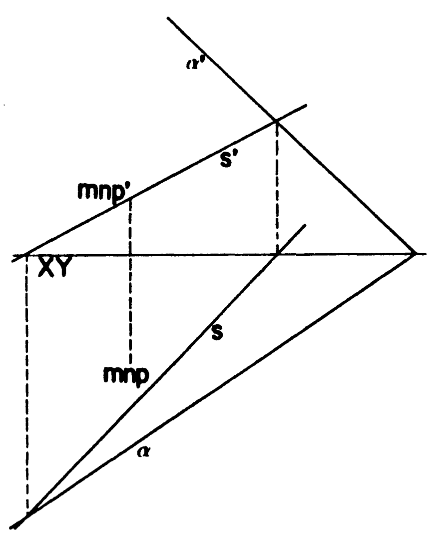

FIG. 4. Point (mnp) not belonging to plane (α).

The other projection of (S) is drawn so that (S) belongs to (α). It is then seen whether the point belongs to the line (S) and, consequently, to the plane (α). In Fig. 5, this process has been applied to the points of the reciprocal space lines $(T_1, T_2 \ldots T_n \ldots T_u)$.

(c) Determination of the true size of plane (α). Two changes of plane are required to bring the plane (α) parallel to one of the coordinate planes. It is assumed that three points A, B, C of the reciprocal lattice belong to (α) (Fig. 5). Figure 6 shows how the new horizontal plane of projections

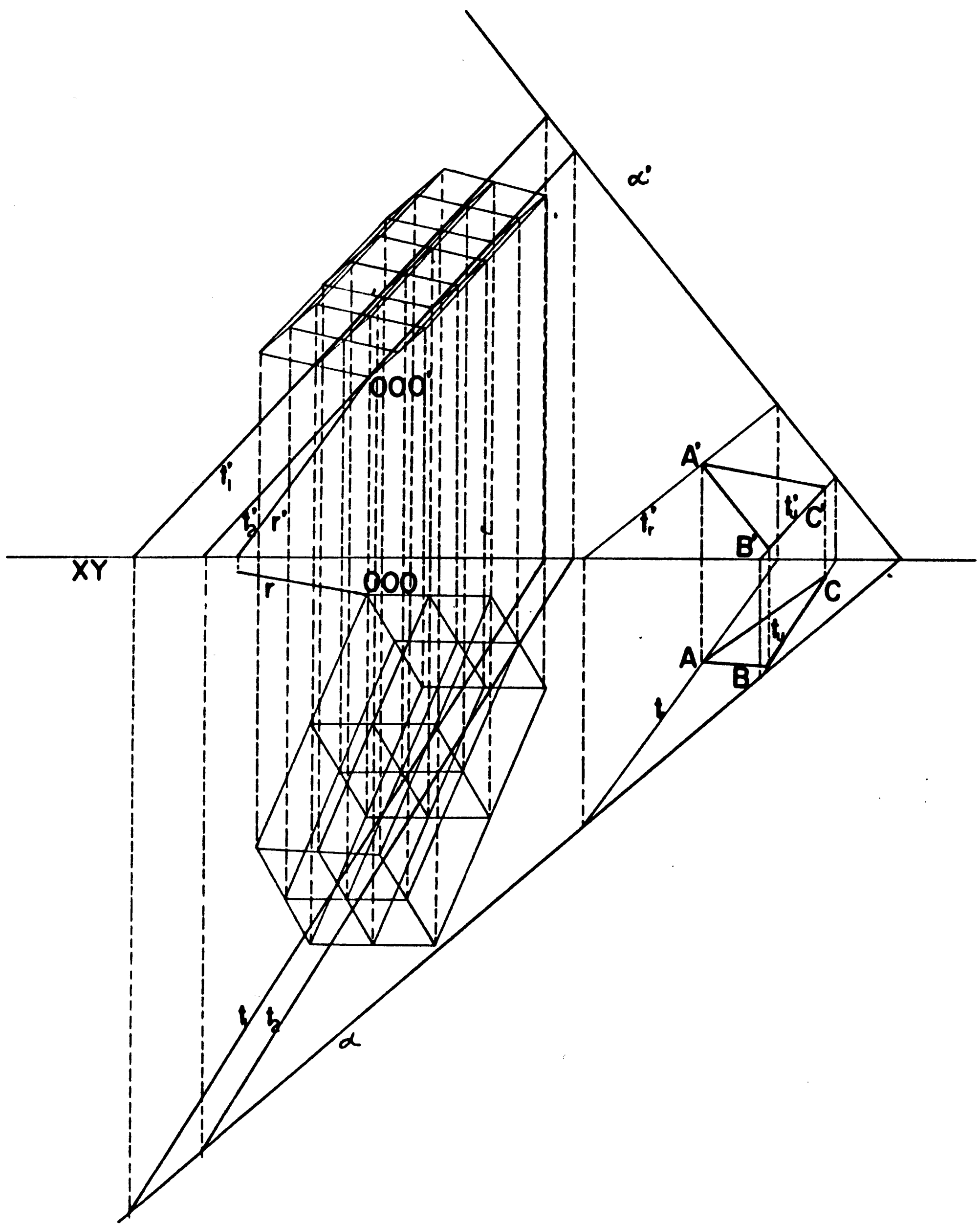

FIG. 5. Determination of the reciprocal lattice points belonging to (α).

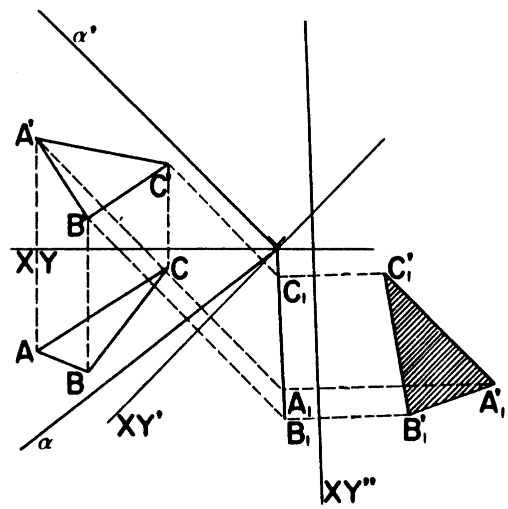

FIG. 6. True size and shape of (ABC).

is drawn in such a way that it is perpendicular to (α). The ground line is shifted to (XY'). For the second change of planes a frontal line in (α) is transformed into a vertical line. The resultant ground line is (XY'') and the vertical plane of projection is parallel to (α). Accordingly, the vertical projection A′B′C′ of ABC is the true size and shape of this triangle.

Application

A typical example will now be introduced; It is required to determine the [22$\bar{1}$] diffraction pattern of a body-centered tetragonal DO_{22} cell, having $a = 3.5$A and $c = 2$a. The simplest sequence of operations is enumerated below

(a) The convenient scale is chosen by means of the camera constant. In reciprocal space;

$$d_{100} = a = \frac{\lambda L}{R_{100}} = \frac{C}{R_{100}} \qquad R_{100} = \frac{C}{a},$$

where d_{100} is the distance between (000) and (100), R_{100} is the distance between center and 100 spot in pattern, C is the camera constant, λ is the electron wavelength.

(b) The allowed reflections are determined from structure factor calculations. In the present example, the allowed ones are $h + k + l$ = even.

(c) The orientation of the reciprocal lattice in relation to the planes of projection is decided upon, as illustrated in Fig. 7.

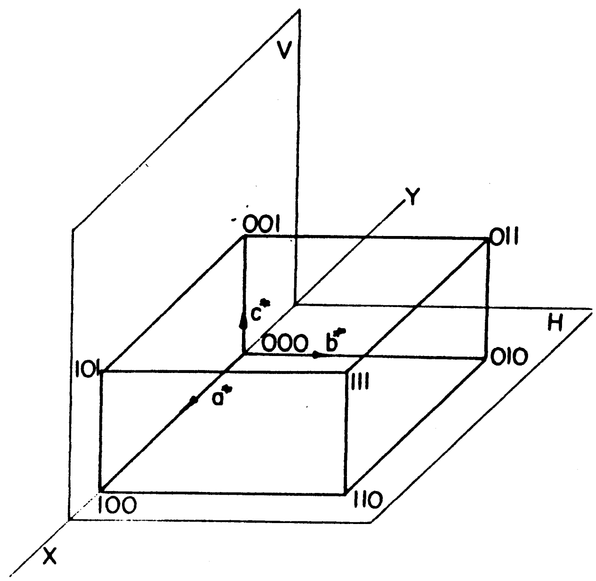

FIG. 7. Orientation of the BCT unit cell in reciprocal space.

(d) The direction of the (*R*) line (representing the incoming beam) is determined in reciprocal space, making use of the property that a line joining reciprocal space points *hkl* and 000 is perpendicular to the (*hkl*) plane in real space. What is then done is to determine the (*hkl*) plane perpendicular to the $[22\bar{1}]$ direction.

Barrett and Massalski [4] provide expressions for the different Bravais lattices. For the tetragonal unit cell

$$\frac{a^2}{h}u = \frac{a^2}{k}v = \frac{c^2}{l}w,$$

and

$$[22\bar{1}] \perp (11\bar{2}).$$

(e) The line joining $11\bar{2}$ and 000 provides the horizontal and vertical projections of the perpendicular to the Ewald plane. In Fig. 8, the Ewald plane is represented by (α). It was already obtained in its "trace" form since 000 is on the ground line.

(f) A series of horizontal lines is passed through the vertical projections of the reciprocal lattice points. These points have received letter indices whenever the periodicity of the lattice and their orientation is such that they represent a whole class of points.

(g) The horizontal projections of the lines are drawn (parallel to the horizontal traces of the plane (α)), and the points that were intercepted

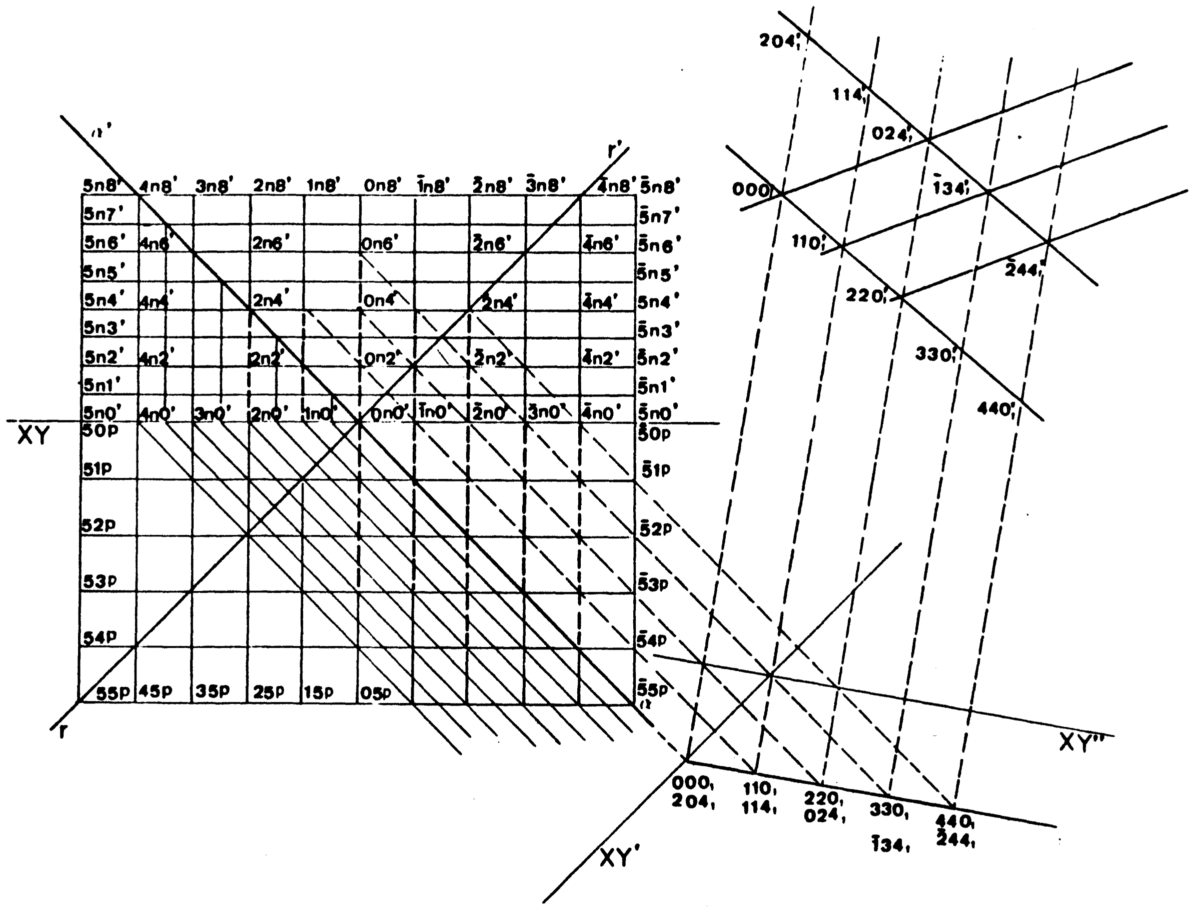

Fig. 8. Typical example.

TABLE 1

Points Belonging to (α)

Vertical Projection	Horizontal Projection
mn6	30p, 21p, 12p, 03p, $\bar{1}$4p
mn4	20p, 11p, 02p, $\bar{1}$3p, $\bar{2}$4p
mn2	10p, 01p, $\bar{1}$2p, $\bar{2}$3p, $\bar{3}$4p
mn0	$\bar{1}$1p, $\bar{2}$2p, $\bar{3}$3p, $\bar{4}$4p

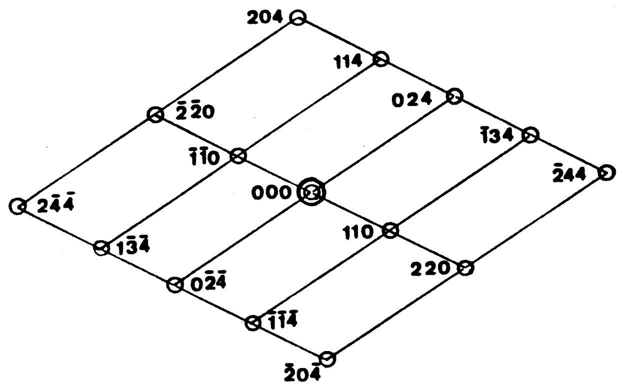

FIG. 9. Resulting diffraction pattern.

are noted, together with their corresponding vertical projections, as shown in Table 1.

The letters m, n, p can be assigned any integral values. The ones that satisfy the above conditions are; 306, 216, 126, 036, $\bar{1}46$, 204, 114, 024, $\bar{1}34$, $\bar{2}44$, 102, 012, $\bar{1}22$, $\bar{2}32$, $\bar{3}42$, $\bar{1}10$, $\bar{2}20$, $\bar{3}30$, $\bar{4}40$.

The conditions for reflection ($h + k + l =$ even) eliminate all but 204, 114, 024, $\bar{1}34$, $\bar{2}44$, $\bar{1}10$, $\bar{2}20$, $\bar{3}30$, $\bar{4}40$.

(h) The above points will be subjected to the two changes of planes previously explained. The ground line is successively changed to (XY') and (XY''), and the resulting pattern is shown in Fig. 8.

(i) Application of the symmetry factors—since only half of the reciprocal lattice was scanned—will provide the other half of the diffraction pattern. This pattern is shown in Fig. 9.

Conclusions

Analytic methods indicate the possible reflections for specific incident beams and the representation of the diffraction patterns can be very laborious since angles and distances have to be determined. It is hoped that this graphical method will introduce simplifications in the determination and indexing of diffraction patterns of more complicated cases. Its main advantage resides in the fact that it leads directly to the pattern.

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References

1. L. E. Murr, *Electron Optical Applications in Materials Science*, McGraw-Hill, New York, 1970, p. 230.
2. A. E. Church and G. M. Bartlett, *Elements of Descriptive Geometry*, American Book Co., New York, 1911, pp. 7-ff.
3. C. H. Schumann, *Descriptive Geometry*, Van Nostrand, New York, 1957, p. 1.
4. C. S. Barrett and T. B. Massalski, *Structure of Metals*, McGraw-Hill, New York, 1966, p. 617.

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