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Indexing of Laue photographs of cubic crystals.

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The simplest method of indexing Laue photographs of a cubic crystal is by the use of the gnomonic projection. If the X-ray beam is incident along, say, the [001] direction, and the plane photographic film is normal to the beam and at a distance D from the crystal, the gnomonic projection will show spots which are found to lie on two sets of parallel lines, the lines of one set being perpendicular to those of the other set. These lines can be labelled

$$h/l = \ldots 4, 3, 2, \tfrac{3}{2}, \tfrac{4}{3}, 1, \tfrac{3}{4}, \tfrac{2}{3}, \tfrac{1}{2}, \ldots, 0, \ldots, -\tfrac{1}{2}, -\tfrac{2}{3}, -\tfrac{3}{4}, -1, \ldots,$$

$$k/l = \ldots 4, 3, 2, \tfrac{3}{4}, \ldots, 0, \ldots, -1, -\tfrac{4}{3}, -\tfrac{3}{2}, -2, \ldots,$$

or, more briefly, $h/l = n/m$ and $k/l = n/m$, where n and m are, in general, *small* positive or negative integers. A spot lying, for example, at the intersection of $h/l = -\frac{5}{3}$ and $k/l = 1$ would have indices $\bar{5}33$. The 'unitary spacing' of either set of lines (distance between lines for which n/m has consecutive integral values, 0 and 1, say) is D. All this is standard practice.

If the X-ray beam is incident along *any* direction $[uvw]$, u, v and w being small integers, the gnomonic projection may be asymmetrical and will appear to be more difficult to index. Provided, however, that parallel rows of spots can be recognized, the indexing can be carried out with ease by a generalization of the rules described above.

Relatively simple zone axes normal to $[uvw]$ will be $[0w\bar{v}]$, $[\bar{w}0u]$, $[v\bar{u}0]$. Planes (hkl) parallel to these zone axes will give projected spots lying on sets of parallel straight lines which may be indexed

$$\frac{kw-lv}{hu+kv+lw} = \frac{n}{m}, \quad \frac{-hw+lu}{hu+kv+lw} = \frac{n}{m}, \quad \frac{hv-ku}{hu+kv+lw} = \frac{n}{m},$$

where n and m are, in general, *small* positive or negative integers. The lines for which $n/m = 0$ will pass through the origin of the projection and are parallel respectively to $[0w\bar{v}]$, $[\bar{w}0u]$ and $[v\bar{u}0]$. They make the following angles with each other, taken in pairs as shown:

$$[0w\bar{v}] : [\bar{w}0u] \text{ at } \cos^{-1}[-uv/\sqrt{\{(w^2+v^2)\,(u^2+w^2)\}}],$$

$$[\bar{w}0u] : [v\bar{u}0] \text{ at } \cos^{-1}[-vw/\sqrt{\{(u^2+w^2)\,(v^2+u^2)\}}], \text{ etc.}$$

Another useful set of lines on the projection is that parallel to $[u'v'w']$, which is normal both to $[uvw]$ and to $[0w\bar{v}]$, so that $uu'+vv'+ww' = wv'-vw' = 0$; this direction is therefore $[-(v^2+w^2)/u, v, w]$, and there are two corresponding directions normal to $[\bar{w}0u]$ and $[v\bar{u}0]$.

More generally still, *any* set of parallel lines on the gnomonic projection can be labelled

$$(hu'+kv'+lw')/(hu+kv+lw) = n/m,$$

where $uu'+vv'+ww' = 0$; and the spacing of the lines for which n/m is integral (the distance from the line 0 to the line 1, say) will be

$$D\sqrt{\{(u^2+v^2+w^2)/(u'^2+v'^2+w'^2)\}}.$$

This fact allows the easy determination of n/m for all such sets of lines.

It is, of course, a very simple matter, once the lines of spots are labelled, to determine hkl for any point on the projection by combining and solving the equations for any two lines on which it occurs, other intersecting lines being used as a check.

Examples

1. *X-ray beam parallel to* [111]

The gnomonic projection shows three sets of lines respectively parallel to $[01\bar{1}]$, $[\bar{1}01]$ and $[1\bar{1}0]$, and at 120° to each other. On these lines lie the projections of planes (hkl) such that

$$\frac{k-l}{h+k+l} = \frac{n}{m}, \quad \frac{l-h}{h+k+l} = \frac{n}{m}, \quad \frac{h-k}{h+k+l} = \frac{n}{m},$$

and the unitary spacing of any of the sets of lines is $D\sqrt{\frac{3}{2}}$. It will be found that another three sets of lines can be drawn at right angles to these; they are parallel to $[\bar{2}11]$, $[1\bar{2}1]$ and $[11\bar{2}]$ respectively and can be indexed $(-2h+k+l)/(h+k+l) = n/m$, etc., the unitary spacing of this set being $D/\sqrt{2}$. A spot lying at the intersection of $(k-l)/(h+k+l) = 1$ and $(-2h+k+l)/(h+k+l) = -\frac{7}{5}$ will have indices $43\bar{2}$, and if the crystal is exactly set, there will be spots $\bar{2}43$ and $3\bar{2}4$ symmetrically placed at the intersections of

$$(l-h)/(h+k+l) = 1 \quad \text{and} \quad (h-2k+l)/(h+k+l) = -\tfrac{7}{5}$$

and of

$$(h-k)/(h+k+l) = 1 \quad \text{and} \quad (h+k-2l)/(h+k+l) = -\tfrac{7}{5}.$$

If the crystal is not exactly set, the lines may not be exactly parallel in each series, and the spacings and angles on the projection will deviate from the ideal, but if the mis-setting is not large the method will still be applicable.

2. *X-ray beam parallel to* $[12\bar{1}]$

The gnomonic projection will show three sets of lines, respectively parallel to [012], [101] and $[2\bar{1}0]$, which can be indexed

$$\frac{k+2l}{h+2k-l} = \frac{n}{m}, \quad \frac{h+l}{h+2k-l} = \frac{n}{m} \quad \text{and} \quad \frac{2h-k}{h+2k-l} = \frac{n}{m}.$$

Their unitary spacings will be $D\sqrt{\frac{6}{5}}$, $D\sqrt{3}$ and $D\sqrt{\frac{6}{5}}$, and the lines in the different sets, taken in pairs, will make angles of $\cos^{-1}\sqrt{\frac{2}{5}}$, $\cos^{-1}\sqrt{\frac{2}{5}}$ and $\cos^{-1}(-\frac{1}{5})$, that is, 50·8, 50·8 and 258·4°, with each other.