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A GENERAL METHOD FOR CALCULATING ELECTRON DIFFRACTION PATTERNS CONTAINING TWIN REFLECTIONS IN ISOMETRIC CRYSTALS

Berkeley, California

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O. Johari and G. Thomas

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A GENERAL METHOD FOR CALCULATING ELECTRON DIFFRACTION PATTERNS CONTAINING TWIN REFLECTIONS IN ISOMETRIC CRYSTALS

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Abstract

A general crystallographic method for calculating twin reflection positions for isometric crystals is described. The usefulness of this method when combined with stereographic projection and electron microscopy techniques are discussed.

Meieran and Richman[1] have proposed a method for the determination of electron diffraction patterns from twinned body-centered cubic crystals. It is the purpose of this note to present a general method capable of predicting the positions of all reflections from both matrix and twin regions for all possible orientations of cubic crystals. The method has been verified for twinning in explosively deformed copper, and is found to be a very useful tool when used in conjunction with stereographic projection, and dark field electron microscopy.

Let an isometric crystal be twinned on any $(hk\ell)$ plane. The twinning can be considered either as a reflection in the twin plane or as a 180° rotation about the twin axis. In reciprocal space, the 180° rotation about the twin axis would place a given point p,q,r, to a new position P,Q,R, such that both will be equally inclined to the twin axis. This is represented in Fig. 1. If the coordinates of three such pairs of points are determined, the matrix of the transformation can be obtained.[2] It is also seen that such pairs would satisfy another condition - i.e., the vector [p,q,r] plus the vector [P,Q,R] will yield a multiple of $hk\ell$, i.e., the indices of the twin plane, because in isometric systems the axis $[hk\ell]$ is perpendicular to the plane $(hk\ell)$.

This can be simplified by taking the points along the three axis. If a point $h^2 + k^2 + \ell^2$, 0, 0 is taken along the x axis, it is seen that its new indices should be $h^2 - k^2 - \ell^2$, $2hk$, $2h\ell$, so as to yield a sum $2h^2$, $2hk$, $2h\ell$, i.e., $2h(h,k,\ell)$. (Also the points $h^2 - k^2 - \ell^2$, $2hk$, $2h\ell$, and $h^2 + k^2 + \ell^2$, 0, 0 are equidistant from the origin and both points make equal angles with the twin axis, i.e., $\cos^{-1}\frac{h}{\sqrt{h^2+k^2+\ell^2}}$). Similar operations for the points, 0, $h^2 + k^2 + \ell^2$, 0 and 0, 0, $h^2 + k^2 + \ell^2$ yield

$2hk$, $k^2 - \ell^2 - h^2$, $2k\ell$, and $2h\ell$, $2k\ell$, $\ell^2 - h^2 - k^2$ respectively after the 180° rotation about the twin axis.

Following the method due to Buerger,[2] the matrix of the transformation is obtained as follows:

$$\begin{vmatrix} \frac{h^2 - k^2 - \ell^2}{h^2 + k^2 + \ell^2} & \frac{2hk}{h^2 + k^2 + \ell^2} & \frac{2h\ell}{h^2 + k^2 + \ell^2} \\ \frac{2hk}{h^2 + k^2 + \ell^2} & \frac{k^2 - \ell^2 - h^2}{h^2 + k^2 + \ell^2} & \frac{2k\ell}{h^2 + k^2 + \ell^2} \\ \frac{2h\ell}{h^2 + k^2 + \ell^2} & \frac{2k\ell}{h^2 + k^2 + \ell^2} & \frac{\ell^2 - h^2 - k^2}{h^2 + k^2 + \ell^2} \end{vmatrix} \text{-------(1)}$$

Using this matrix the indices of any other point in reciprocal space can be determined.

This matrix is much simplified for {111} twinning commonly encountered in fcc metals, since $h^2 + k^2 + \ell^2 = 3$, and $h^2 - k^2 - \ell^2$, $k^2 - \ell^2 - h^2$, and $\ell^2 - h^2 - k^2$ are each equal to -1,

hence $$P = \frac{(-p + 2hkq + 2h\ell r)}{3}$$

or $$P = \frac{(-hp + 2kq + 2\ell r)}{3h}$$

$$Q = \frac{(2hp - kq + 2\ell r)}{3k}$$

$$R = \frac{(2hp + 2kq - \ell r)}{3\ell}$$

where $(hk\ell)$ stands for any of the {111} planes. This formula can be used to find both the positions of spots after twinning and the orientation of twinned regions if the matrix orientation is known. In electron microscopy this orientation can be found from the diffraction pattern.

Similarly for {112} twinning, commonly encountered in bcc metals, the transformation is given by:

$$P = \frac{\{(h^2 - k^2 - \ell^2)p + 2hkq + 2h\ell r\}}{6}$$

$$Q = \frac{\{2hkp + (k^2 - \ell^2 - h^2)q + 2k\ell r\}}{6}$$

$$R = \frac{\{2h\ell p + 2k\ell q + (\ell^2 - h^2 - k^2)r\}}{6}$$

which is a more general formula than that given by Meieran and Richman[1] in that it includes all {112} planes.

The transformation obtained by matrix (1) corresponds to a rotation of 180° about the twin axis. If the twinning is regarded as reflection in the twin plane the result should be modified by multiplying the matrix (1) by the following:

$$\begin{vmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{vmatrix} \qquad \text{----------(2)}$$

since in crystallography $A_{\pi} + \bar{1} = m$.

In transmission electron microscopy, although exact foil orientations can be determined by indexing Kikuchi lines, often only spot patterns are observed. In the latter case the orientation can only be approximately found. However, if a projection of the approximate orientation is drawn, the position of spots from twinned regions can be determined by reflection along the twinning plane or by 180° rotation about the twin axis. If the twinned spots fall on, or close to the basic circle of the standard projection, they are likely to appear on the diffraction pattern. The experimental and calculated diffraction patterns can then be correlated. It should be

noted that when multiple twinning occurs double diffraction becomes important and should be accounted for.[3]

It should also be pointed out that twin and matrix reflections coincide for certain orientations so that no extra reflections may be observed. Examples for (001) and (110) fcc are shown in Fig. 2. In electron microscopy investigations of mechanical twinning and twinned martensite it is important to recognize this fact, i.e., the absence of extra reflections should not be taken as indicating the absence of twinning until the twin positions have been verified. Dark field experiments are extremely helpful to show if twinning is present, e.g., from Fig. 2(a) it can be seen that the dark field image of the 220 type reflection will reverse contrast from twins whereas the dark field image of the 200 type reflection will not.[3]

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References

1. E. S. Meieran and M. H. Richman, Trans AIME 227, 1044 (1963).

2. M. J. Buerger, X-Ray Crystallography, John Wiley & Sons, New York, 1942, p. 10.

3. O. Johari and G. Thomas, to be published. Also University of California Lawrence Radiation Laboratory Report UCRL-10932 (1963).

Figure Captions

Fig. 1. Sketch showing the twin position P,Q,R, of a reciprocal lattice point p,q,r, obtained by a 180° rotation about the twin axis [hkℓ].

Fig. 2. (a) Expected diffraction pattern by twinning on {111} planes for (001) orientation. The orientation of twinned crystal becomes {221}.

(b) Expected diffraction pattern by twinning on (111) plane for (110) orientation. The orientation of twinned crystal becomes $(\bar{1}\bar{1}4)$.

For both cases no extra spots appear and the spots from the twinned material overlap those from the matrix.

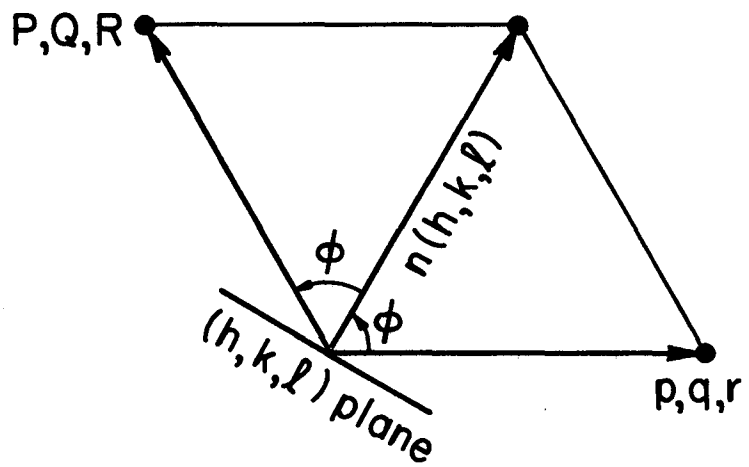

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Fig. 1

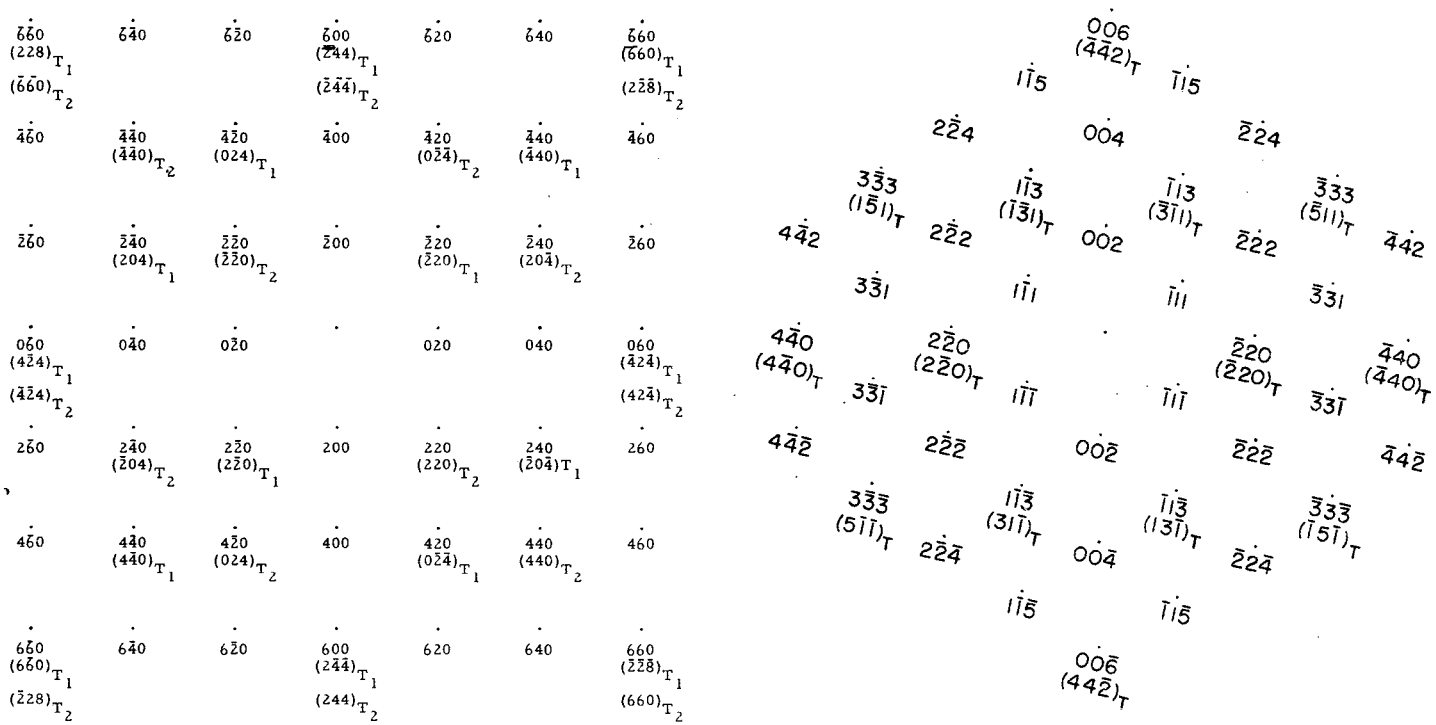

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Fig. 2

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