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The Calculation of Electron Diffraction
Patterns Containing Twin Reflections

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by

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Abstract

The positions of twin reflections in electron diffraction patterns obtained from thin metal foils may be calculated for any twin in any crystal structure by means of an elementary application of vector algebra. General equations for the four classical orientation relationships are presented using the superscript and subscript notation of the tensor calculus, which is briefly described. As an example of the application of these expressions, the case of twinned rhombohedral crystals, and hence as a special case, twinned cubic crystals, is examined.

Considerable interest has recently been shown in the interpretation of electron diffraction patterns obtained from twinned regions of thin metal foils. In the present paper, it is shown that the necessary information may be obtained directly for all twins in any crystal structure by means of a very elementary application of vector algebra. The equations involved are most conveniently presented by making use of the very powerful superscript and subscript notation of the tensor calculus. The use of this notation will first be described and then applied to the problem of calculating diffraction patterns for any twinned crystal. Finally, as an example of the application of the method, the specific case of twinned rhombohedral crystals will be considered.

The Tensor Notation

The triplet of primitive lattice vectors defining the edges of a cell of the direct lattice will be represented by $\underline{a}_i$. (Here, as elsewhere in this paper, letters occurring as subscripts or superscripts may take the values 1, 2, or 3.) The corresponding triplet of vectors defining a cell of the reciprocal lattice will then be given by $\underline{a}^i$ and these two bases will be related by the equation $\underline{a}_i \cdot \underline{a}^j = \delta_i^j$, where $\delta_i^j = 1$ when $i=j$ and otherwise is zero. Relations between vectors representing directions and plane normals are most conveniently written by making use of the metric tensors a_{ij} and a^{ij} of the bases $\underline{a}_i$ and $\underline{a}^i$ respectively are defined by the equations

$$a_{ij} = \underline{a}_i \cdot \underline{a}_j \quad \text{and} \quad a^{ij} = \underline{a}^i \cdot \underline{a}^j \quad (a)$$

Each may be written as a 3x3 array. Thus for example,

$$a_{ij} = \begin{pmatrix} \underline{a}_1 \cdot \underline{a}_1 & \underline{a}_1 \cdot \underline{a}_2 & \underline{a}_1 \cdot \underline{a}_3 \\ \underline{a}_2 \cdot \underline{a}_1 & \underline{a}_2 \cdot \underline{a}_2 & \underline{a}_2 \cdot \underline{a}_3 \\ \underline{a}_3 \cdot \underline{a}_1 & \underline{a}_3 \cdot \underline{a}_2 & \underline{a}_3 \cdot \underline{a}_3 \end{pmatrix}$$

We may now write

$$\underline{a}_i = a_{ik} \underline{a}^k \quad (b)$$

where, as elsewhere, indices occurring twice in an expression (always once as a subscript and once as a superscript) are to be summed over the values 1, 2, and 3 so that, for example, letting $i=1$ in equation (b), $\underline{a}_1 = a_{11}\underline{a}^1 + a_{12}\underline{a}^2 + a_{13}\underline{a}^3$. Taking the scalar product of both sides of equation (b) with $\underline{a}_j$, we obtain, using equation (a), the identity $a_{ij} = a_{ik} \delta_j^k (= a_{ij})$. Also since $\underline{a}^i = a^{ij} \underline{a}_j$ the scalar product of $\underline{a}_i$ and $\underline{a}^i$ now gives us $a_{ip} a^{jp} = \delta_i^j$. The array a^{ij} may thus be obtained by inverting the array a_{ij} as in matrix algebra.

Vectors representing lattice directions are normally resolved into components using the direct lattice basis. The components of a given direction

will be represented by an italic letter with a superscript. Similarly, the Miller indices of a plane are the components of the vector normal to the plane resolved in the reciprocal basis and are represented by an italic letter with a subscript. By substituting for $\underline{a}_i$ and $\underline{a}^i$ it is readily seen that the vector $u^i \underline{a}_i$ representing the direction u^i and the vector $h_j \underline{a}^j$ representing the plane h_j may be written $a_{ij} u^i \underline{a}^j$ and $a^{ij} h_j \underline{a}_i$ respectively. Using this notation the scalar product of the two vectors $u^i \underline{a}_i$ and $h_j \underline{a}^j$ is $u^i h_j \delta_i^j = u^i h_i$. It follows that the scalar product

of the two vectors $u^i \underline{a}_i$ and $v^j \underline{a}_j$ is given by $a_{ij} u^i v^j$ and of the two vectors $h_i \underline{a}^i$ and $k_j \underline{a}^j$ by $a^{ij} h_i k_j$.

The General Expressions

In this paper the four classical orientation relationships associated with deformation twinning will be considered⁽⁴⁾. These are obtained by:

- (i) Reflection in the twinning plane K_1 ,
- (ii) Rotation of π about the normal to K_1 ,
- (iii) Rotation of π about the twinning direction η_1 ,
- (iv) Reflection in the plane normal to η_1 .

Relationships (i) and (ii) are associated with Type I twinning in which the K_1 plane has rational Miller indices and relationships (iii) and (iv) with Type II twinning in which η_1 is rational. Electron diffraction patterns arising from twinned metal foils obeying other possible orientation relationship laws are at present being examined and will be discussed elsewhere

The four orientation relationships given above are illustrated schematically as diagrams (i) to (iv) of Fig. 1. In this figure $\underline{h}$ and $\underline{u}$ are vectors normal to K_1 and parallel to η_1 respectively, and $\underline{c}$ and $\underline{p}$ represent the normals to twin related planes, the plane $\underline{c}$ being considered to lie in the matrix. Using these diagrams, we can immediately write the following vector equations for the four orientation relationships:

$$\underline{p}^{(i)} = \underline{c} - 2(\underline{c} \cdot \underline{h})(\underline{h} \cdot \underline{h})^{-1} \underline{h} \quad (1)$$

$$\underline{p}^{(ii)} = -\underline{c} + 2(\underline{c} \cdot \underline{h})(\underline{h} \cdot \underline{h})^{-1} \underline{h} \quad (2)$$

$$\underline{p}^{(iii)} = -\underline{c} + 2(\underline{c} \cdot \underline{u})(\underline{u} \cdot \underline{u})^{-1} \underline{u} \quad (3)$$

$$\underline{p}^{(iv)} = \underline{c} - 2(\underline{c} \cdot \underline{u})(\underline{u} \cdot \underline{u})^{-1} \underline{u} \quad (4)$$

Equations (1) to (4) illustrate the well-known result ⁽³⁾ that, for centrosymmetric structures, relationships (i) and (ii) are equivalent, as are relationships (iii) and (iv).

In order to write equations (1) to (4) in terms of Miller indices, we make use of the tensor notation. Thus, directions and planes will be referred to the direct and reciprocal lattice bases, $\underline{a}_i$ and $\underline{a}^i$, of the matrix crystal and the vectors $\underline{u}$, $\underline{h}$, $\underline{c}$, and $\underline{p}$ will be represented by u^i , h_i , c_i , and p_i respectively. Thus, we obtain

$$\pm p_i^{(I)} = c_i - 2(a^{ij} c_j h_i)(a^{ij} h_i h_j)^{-1} h_i \quad (5)$$

for Type I twinning and

$$\pm p_i^{(II)} = c_i - 2(c_i u^i)(a_{ij} u^i u^j)^{-1} a_{ij} u^j \quad (6)$$

for Type II twinning.

In metals many of the possible twinning modes, and indeed nearly all of the observed modes ⁽³⁾, have both K_1 and η_1 rational, so that the orientation relationships associated with both types of twinning may be applicable. Furthermore, if the plane of shear, which is defined as the plane containing the vectors $\underline{h}$ and $\underline{u}$, is a mirror plane, as it is in most twinning modes in metals ⁽³⁾, the two planes $p_i^{(I)}$ and $p_i^{(II)}$ defined by equations (5) and (6) are crystallographically equivalent.

Spots on electron diffraction patterns from thin foil specimens only arise from planes which are approximately parallel to the electron beam. Thus, if the beam is parallel to a direction v^i in the

matrix crystal, a spot corresponding in the twin crystal to a plane, which is parallel to a plane p_i of the matrix and twin related to a plane c_i of the matrix, will only arise if the scalar product $p_i v^i$ is approximately zero. Thus, for a foil of known crystallographic orientation relative to the electron beam, the diffraction pattern expected from a twinned region may be readily determined using equations (5) and (6).*

A Specific Application

In order to illustrate the use of equations (5) and (6) and of the tensor notation being employed, the specific example of twinning in rhombohedral crystals, and hence as a special case in cubic crystals, will now be examined. Letting the direct lattice be defined by a rhombohedral cell of angle α and with unit edges, we obtain

$$a_{ij} = \begin{pmatrix} 1 & \cos \alpha & \cos \alpha \\ \cos \alpha & 1 & \cos \alpha \\ \cos \alpha & \cos \alpha & 1 \end{pmatrix}$$

and

$$a^{ij} = (1 + \cos \alpha - 2\cos^2 \alpha)^{-1} \begin{pmatrix} 1 + \cos \alpha & -\cos \alpha & -\cos \alpha \\ -\cos \alpha & 1 + \cos \alpha & -\cos \alpha \\ -\cos \alpha & -\cos \alpha & 1 + \cos \alpha \end{pmatrix}$$

so that equations (5) and (6) give

$$\pm(p_1^{(I)}, p_2^{(I)}, p_3^{(I)}) = (c_1, c_2, c_3) - 2A(h_1, h_2, h_3) \quad (7)$$

where

$$A = \frac{(1 + \cos \alpha)(c_1 h_1 + c_2 h_2 + c_3 h_3) - \cos \alpha(c_1 h_2 + c_1 h_3 + c_2 h_3 + c_2 h_1 + c_3 h_1 + c_3 h_2)}{(1 + \cos \alpha)(h_1^2 + h_2^2 + h_3^2) - 2\cos \alpha(h_1 h_2 + h_2 h_3 + h_3 h_1)}$$

* The actual calculation of diffraction patterns from equations (5) and (6) is a routine procedure; a detailed example for a twinned body centred cubic crystal has been given by Meieran and Richman⁽¹⁾.

and

$$\pm(p_1^{(II)}, p_2^{(II)}, p_3^{(II)}) = (c_1, c_2, c_3) - 2B \left(u^1 + \cos \alpha (u^2 + u^3), u^2 + \cos \alpha (u^3 + u^1), u^3 + \cos \alpha (u^1 + u^2) \right) \quad (8)$$

where

$$B = \frac{c_1 u^1 + c_2 u^2 + c_3 u^3}{\left((u^1)^2 + (u^2)^2 + (u^3)^2 \right) + 2 \cos \alpha (u^1 u^2 + u^2 u^3 + u^3 u^1)}$$

Thus, for example, the reported twinning mode ⁽³⁾ of the rhombohedral metals mercury, bismuth, antimony, and arsenic has $K_1 = (110)$ and $\gamma_1 = [001]$, when the face centred rhombohedral cell is used, so that the plane of shear is the mirror plane $(1\bar{1}0)$ and we obtain from equations (7) and (8) the following two crystallographically equivalent forms of p_i

$$\pm p_1^{(I)} = (-c_2 + 2c_3 \cos \alpha, -c_1 + 2c_3 \cos \alpha, c_3)$$

$$\pm p_1^{(II)} = (c_1 - 2c_3 \cos \alpha, c_2 - 2c_3 \cos \alpha, -c_3)$$

In cubic crystals we have $\alpha = \pi/2$ so that

$$a_{ij} = a^{ij} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and equations (7) and (8) then reduce to the form given in references (1) and (2). Using the tensor notation, we may write these equations in the condensed form

$$\pm p_1^{(I)} = c_i - 2(c_i h_i)(h_i h_i)^{-1} h_i \quad (9)$$

$$\pm p_1^{(II)} = c_i - 2(c_i u^i)(u^i u^i)^{-1} u^i \quad (10)$$

The value of employing the powerful notation offered by the tensor calculus is particularly evident when equations (9) and (10) are compared with the equivalent lengthy expressions given by previous workers^(1, 2) who considered cubic crystals exclusively.

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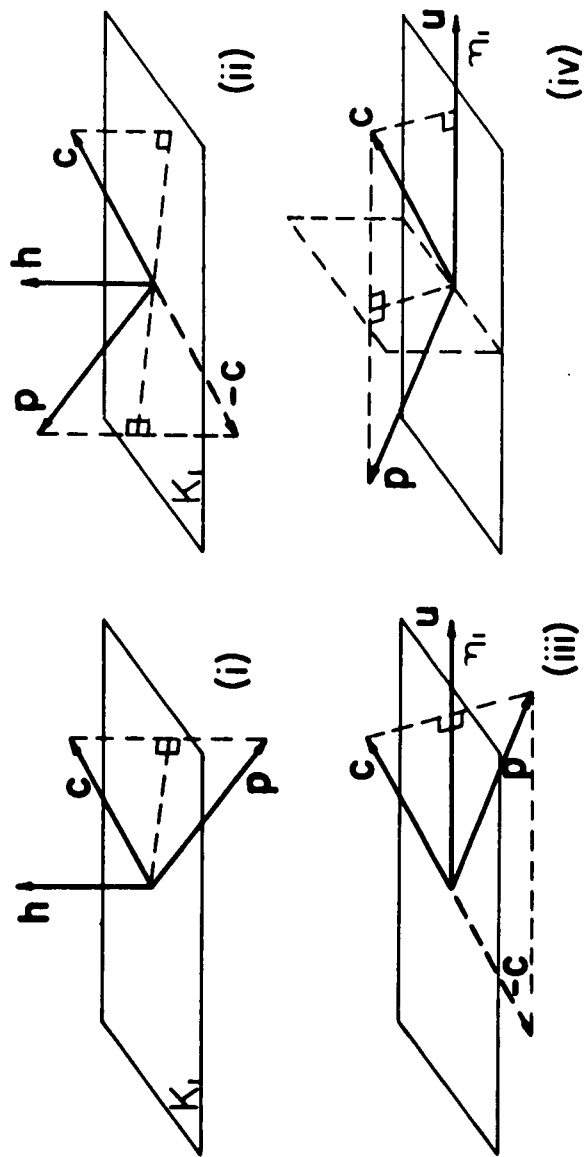


Figure 1. The four classical orientation relationships of deformation twinning. The vectors h and u represent the normal to the twinning plane K_1 , and the twinning direction l_1 , respectively. The planes normal to the vectors c and p are twin related in all four cases.

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