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Orientation Relationships Between Two Crystal Lattices: Matrix Description

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Abstract

Orientation relationships between two crystal lattices are frequently specified in terms of parallel directions and planes in each lattice. The corresponding matrix, relating the vector bases of the lattices, can be obtained by a general method involving the metric matrices of the two lattices and the crystallographic indices of parallel planes and directions. Equivalent matrices can be defined by changing the lattice bases: different selections of the invariants of such matrices are indicated. Finally, criteria for choosing the 'best' matrix relating the two lattices are discussed in the context of phase transformations and of interfacial structure.

1. Introduction

There are various situations where it is of interest to specify the relative orientation of two crystal lattices; for example, when the two crystals meet at an interface or when one of the crystals is phase transformed into the other. Frequently, the relative orientation is defined by indicating the crystallographic indices of planes or directions, in each lattice, that are parallel to each other. The possibilities are: two pairs of parallel directions; two pairs of parallel planes; one pair of directions and one pair of planes, this being the more commonly used. However, the most convenient and formally simpler way of specifying the relative orientation of two lattices with bases $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \equiv (\mathbf{e})$ and $(\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3) \equiv (\mathbf{e}')$, respectively, is in terms of the 3×3 matrix X that relates the two bases:

$$[\mathbf{e}'_1\ \mathbf{e}'_2\ \mathbf{e}'_3] = [\mathbf{e}_1\ \mathbf{e}_2\ \mathbf{e}_3]X \qquad (1)$$

or

$$\mathbf{e}' = \mathbf{e}X. \qquad (2)$$

In these equations, $[\mathbf{e}_1\ \mathbf{e}_2\ \mathbf{e}_3] \equiv \mathbf{e}$ is to be regarded as a row matrix. When the orientation matrix X is known, one can determine the angles between any directions or planes in the two lattices and find a correlation between the lattices in terms of the product of a pure rotation and a pure deformation (*e.g.* Christian, 1975). One can also study the possibility of coincident points between the two lattices and whether such points define a three-, two- or one-dimensional lattice and determine the degree of coincidence in each case. Methods of solving these problems have been developed by Grimmer (1976) and Fortes (1983*b*). Finally, it is possible to determine the 0-lattice from the matrix X (Bollman, 1970) and calculate the misfit dislocation content of an interface between the two crystals (Bollmann, 1970; Knowles, 1982).

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In this paper we develop a method for determining the matrix X from the parallelism of directions and planes, and discuss the special matrices equivalent to X that can be selected to characterize the relative orientation.

2. Determination of the orientation matrix

Suppose that two directions, defined by their crystallographic indices in each lattice, are parallel:

$$[h_1\ h_2\ h_3] \| [h'_1\ h'_2\ h'_3]. \tag{3}$$

To treat the more complicated and more common case suppose that, in addition, the following planes, defined by their Miller indices in each lattice, are parallel

$$(u_1\ u_2\ u_3) \| (u'_1\ u'_2\ u'_3). \tag{4}$$

From the known bases (**e**) and (**e**′) of the two lattices we obtain the metric matrices G, G'. For example, $G=(g_{ij})$ with $g_{ij}=\mathbf{e}_i.\mathbf{e}_j$. It may be useful to express the bases in an orthonormal reference system, $(\mathbf{o}_1\ \mathbf{o}_2\ \mathbf{o}_3)$. For example, for the basis (**e**):

$$\mathbf{e}=\mathbf{o}P$$

and

$$G=P^TP,$$

where P^T is the transpose of P. The reciprocal lattices have bases (**r**), (**r**′), respectively, defined by

$$\begin{aligned}\mathbf{r}&=\mathbf{e}G^{-1}\\ \mathbf{r}'&=\mathbf{e}'G'^{-1},\end{aligned} \tag{5}$$

where, as before, $\mathbf{r}=[\mathbf{r}_1\ \mathbf{r}_2\ \mathbf{r}_3]$. The reciprocal bases are related by

$$\mathbf{r}'=\mathbf{r}(X^T)^{-1}. \tag{6}$$

Denoting by $h=\{h_i\}$ a column vector with elements h_1, h_2, h_3, (3) is equivalent to

$$\mathbf{e}h=\lambda\mathbf{e}'h' \tag{7}$$

where λ is a real number which relates the moduli of the two vectors. Since the square of the modulus of $\mathbf{h}=\mathbf{e}h$ is h^TGh, λ can be determined from

$$h^TGh=\lambda^2h'^TG'h'. \tag{8}$$

Relation (4) can be written in terms of vectors of the reciprocal lattices:

$$\mathbf{r}u=\mu\mathbf{r}'u' \tag{9}$$

because the vector $\mathbf{u}=\mathbf{r}u$ is perpendicular to the plane with indices $(u_1\ u_2\ u_3)$; u is a column vector with elements u_1, u_2, u_3. Since G^{-1} is the metric matrix of the reciprocal lattice (**r**), μ is determined from

$$u^TG^{-1}u=\mu^2u'^TG'^{-1}u'. \tag{10}$$

Both λ and μ can be taken as positive. Note that $h^Tu=h'^Tu'=0$.

Combining (2) with (7) and (5) with (9) we obtain the following equations for X:

$$h=\lambda Xh' \tag{11}$$

$$u=\mu(X^T)^{-1}u'. \tag{12}$$

These equations can be written in the equivalent form

$$Xh'=(1/\lambda)h \tag{13}$$

$$XG'^{-1}u'=(1/\mu)G^{-1}u, \tag{14}$$

where, for the last equation, we have used the relation $X^T=G'X^{-1}G^{-1}$.

We introduce two vectors **k** and **k**′, with components k and k' in the bases (**e**) and (**e**′), respectively, such that

$$\begin{aligned}G^{-1}u&=k\\ G'^{-1}u&=k'.\end{aligned} \tag{15}$$

The vectors **k** and **k**′ are parallel by virtue of (14).

Now, if **a** and **b** are two vectors of a lattice (**e**), their cross product can be determined from the symbolic determinant rule as

$$\mathbf{a}\times\mathbf{b}=\Omega\begin{vmatrix}\mathbf{r}_1 & \mathbf{r}_2 & \mathbf{r}_3\\ a_1 & a_2 & a_3\\ b_1 & b_2 & b_3\end{vmatrix}. \tag{16}$$

where

$$\Omega=(\det G)^{1/2}. \tag{17}$$

Using this rule we may calculate the cross products

$$\begin{aligned}\mathbf{y}&=\mathbf{h}\times\mathbf{k}\\ \mathbf{y}'&=\mathbf{h}'\times\mathbf{k}'.\end{aligned} \tag{18}$$

Since the vectors **h**, **h**′ and **k**, **k**′ are parallel, **y** is parallel to **y**′ and we write

$$\mathbf{r}\mathbf{y}=\xi\mathbf{r}'\mathbf{y}' \tag{19}$$

with

$$\xi=\mu\lambda\Omega'/\Omega. \tag{20}$$

Comparing this with (9) and (14) we may obtain from (19)

$$XG'^{-1}y'=(1/\xi)G^{-1}y, \tag{21}$$

which, together with (13) and (14),

$$Xh'=(1/\lambda)h \tag{13}$$

$$XG'^{-1}u'=(1/\mu)G^{-1}u, \tag{14}$$

completely determine X. In order to obtain X explicitly we construct two matrices M and M', the columns of which are, in the same order, the column vectors in the second and first members, respectively, of (13), (14) and (21), that is, symbolically

$$M=\left(\frac{1}{\lambda}h\quad \frac{1}{\mu}G^{-1}u\quad \frac{1}{\xi}G^{-1}y\right) \tag{22}$$

$$M'=(h'\quad G'^{-1}u'\quad G'^{-1}y'). \tag{23}$$

We then have

$$X = MM'^{-1}. \tag{24}$$

To summarize, the matrix X relating the two lattice bases can be determined as follows:

1. Calculate λ (for directions) and μ (for planes), respectively, from (8) and (10).
2. For planes, determine the vectors **k** and **k'** from (15).
3. Determine the cross products **y**, **y'** from (16) and the value ξ from (20).
4. Construct the matrices M, M' as defined in (22) and (23).
5. Obtain X from (24).

If the relative orientation is defined by the parallelism of two pairs of directions or two pairs of planes, the alterations that have to be made in the method are obvious.

3. Example of application

The relative orientation between austenite and ferrite in the martensitic transformation in steels is frequently defined by the relations (Kurdjumov & Sachs, 1930)

$$(111)_a \| (110)_f$$

$$[1\bar{1}0]_a \| [1\bar{1}1]_f.$$

These indices are referred to conventional cubic bases in both lattices, (**a**) and (**f**), with lattice parameters α and φ, respectively for austenite and ferrite. If the volume change is negligible,

$$\alpha/\varphi = 2^{1/3}.$$

We follow the various steps outlined above, identifying (**e**) with austenite, to find the matrix X in

$$\mathbf{f} = \mathbf{a}X.$$

Note that $G = \alpha^2 I$ and $G' = \varphi^2 I$ where I is the identity matrix.

1.
$$\lambda = (2/3)^{1/2}(\alpha/\varphi); \qquad \mu = (3/2)^{1/2}(\varphi/\alpha).$$

2.
$$k = \frac{1}{\alpha^2}\begin{bmatrix}1\\1\\1\end{bmatrix} \qquad k' = \frac{1}{\varphi^2}\begin{bmatrix}1\\1\\0\end{bmatrix}.$$

3.
$$y = \alpha\begin{bmatrix}-1\\-1\\2\end{bmatrix} \qquad y' = \varphi\begin{bmatrix}-1\\1\\2\end{bmatrix}; \qquad \xi = \varphi^3/\alpha^3.$$

4.
$$M = \begin{bmatrix} \left(\frac{3}{2}\right)^{1/2}\frac{\varphi}{\alpha} & \left(\frac{2}{3}\right)^{1/2}\frac{1}{\varphi\alpha} & -\frac{\alpha^2}{\varphi^3} \\ -\left(\frac{3}{2}\right)^{1/2}\frac{\varphi}{\alpha} & \left(\frac{2}{3}\right)^{1/2}\frac{1}{\varphi\alpha} & -\frac{\alpha^2}{\varphi^3} \\ 0 & \left(\frac{2}{3}\right)^{1/2}\frac{1}{\varphi\alpha} & \frac{2\alpha^2}{\varphi^3} \end{bmatrix}$$

$$M' = \begin{bmatrix} 1 & 1/\varphi^2 & -1/\varphi \\ -1 & 1/\varphi^2 & 1/\varphi \\ 1 & 0 & 2/\varphi \end{bmatrix}.$$

5.
$$X = \frac{1}{(6d)^{2/3}}\begin{bmatrix} 2d+1 & -1 & d-2 \\ 1 & 2d-1 & -d-2 \\ d-2 & d+2 & 4 \end{bmatrix};$$

$$d = 6^{1/2}\left(\frac{\varphi}{\alpha}\right)^3.$$

If, instead of conventional bases, we had used (true) primitive bases for both lattices, the matrix relating these bases could easily be obtained from X. In either case, the orientation matrices are not rational, implying that the two lattices are not in a coincidence site lattice orientation (*e.g.* Fortes, 1983*b*). However, for particular values of φ/α, coincidence can occur in one direction (but not in two directions, *i.e.* on a plane). For example, if φ/α is rational, coincidence occurs in the direction $[\bar{1}12]_f$, which is parallel to $[11\bar{2}]_a$, but the density of coincidence sites will be very small for the usual values of φ/α. It is therefore unlikely that coincidence of lattice sites in the two crystals plays any role in the phase transformation.

4. Equivalent descriptions

The matrix X obtained by the method of §2 refers to the particular bases (**e**) and (**e'**) in the two lattices used to specify the indices of planes and directions that are palallel. Let us now take new bases $\tilde{\mathbf{e}}$ and $\tilde{\mathbf{e}}'$ related to the original bases by

$$\begin{aligned} \tilde{\mathbf{e}} &= \mathbf{e}T \\ \tilde{\mathbf{e}}' &= \mathbf{e}'T'. \end{aligned} \tag{25}$$

The matrices T and T' have integral coefficients and the absolute value of their determinants is unity. Such matrices can be termed l-matrices (Fortes, 1983*a*). The transformation between the two lattices is now described by a matrix $\tilde{X}$ related to the original matrix X by

$$\tilde{X} = T^{-1}XT'; \qquad \tilde{\mathbf{e}}' = \tilde{\mathbf{e}}\tilde{X}. \tag{26}$$

Note that T^{-1} is also a l-matrix.

We shall discuss the two following questions: (i) what do the various equivalent matrices $\tilde{X}$ have in common?; (ii) what criteria can be used to choose a particular matrix $\tilde{X}$?

The transformation X between the two lattices can be decomposed in the product of a deformation, D, and a rotation, R

$$X = RD. \tag{27}$$

The determination of R and D is discussed by Christian (1975). The rotation can be specified by an axis/angle pair (involving three scalar parameters) and the deformation by indication of the principal strain directions (three parameters) and values (three parameters). These nine parameters are in general invariant in a change of bases and can be used to characterize the relative orientation. When the lattices admit symmetry rotations, there are matrices T and T' that are rotation matrices; the axis/angle pair is not invariant in such cases. Grimmer (1980) developed a method that allows a unique description of the relative rotation for two identical lattices.

When the matrix X is rational (rational elements) it can be put in a diagonal form by a change of bases (Fortes, 1983*a*). Since any matrix can be approximated by a rational matrix, the diagonalization is possible in all cases. It implies the parallelism of three pairs of lattice directions with commensurate identity distances in each pair. These directions can be specified by six parameters which together with the values of the diagonal elements completely define the relative orientation.

Knowles (1982) and Knowles & Smith (1982) have reviewed and discussed the various possibilities of choice of the transformation matrix which are relevant to the determination of the structure and properties of crystalline interfaces. In this case, the important quantities are those related to the misfit dislocation content of the interface.

When dealing with phase transformations other types of criteria are usually introduced, related to the decomposition of the orientation matrix in rotation and deformation (Christian, 1975; Dahmen, 1982). An alternative criterion is to choose a matrix $\tilde{X}$ that relates nearest neighbours in the two lattices. This has been discussed by Bollmann (1970) but some points of his analysis need clarification.

Assuming that the two lattices have a common point 0, we take primitive cells in each lattice with the common corner 0 and with a correspondence defined by a matrix X. Pairs of corresponding points, i, in two lattices have their relative positions defined by vectors $\mathbf{t}_i$. The problem consists of finding the unit cells and the matrix X that minimizes some 'proximity' function of the $\mathbf{t}_i$ for the pairs of points in a specified region including 0. This function may simply be the sum of the moduli of the vectors $\mathbf{t}_i$ for the eight corners of the unit cells at 0. Methods of solving this particular problem were delineated by Bollmann (1970). A more general approach along this line would be to allow for a relative rigid-body translation of the two lattices, $\mathbf{t}_0$, and minimize a proximity function of $\mathbf{t}_i + \mathbf{t}_0$ with respect to the bases and to the translation $\mathbf{t}_0$.

An alternative criterion of proximity is to consider the volume of the parallelepiped defined by the three vectors $\mathbf{t}_i$ relative to the end points of the base vectors:

$$\mathbf{t}_i = \tilde{\mathbf{e}}'_i - \tilde{\mathbf{e}}_i = \tilde{e}_i(\tilde{X} - I) = \tilde{e}'_i(I - \tilde{X}^{-1}) \quad (i = 1, 2, 3). \tag{28}$$

This then leads to the following equivalent conditions for $\tilde{X}$:

$$|\det(\tilde{X} - I)| \quad \text{or} \quad |\det(I - \tilde{X}^{-1})| \quad \text{minimum.} \tag{29}$$

The latter condition was given by Bollmann (1970) but he did not give a method for determining $\tilde{X}$. From (26) and with the fact that the product of two 1-matrices is a 1-matrix, (29) is equivalent to finding a 1-matrix U such that

$$|\det(X - U)| \quad \text{minimum.} \tag{30}$$

Any decomposition of U in the form $U = TT'^{-1}$ gives the required matrix $\tilde{X} = T^{-1}XT'$. A unique decomposition exists if one of the bases is fixed. It may happen that the minimum value of (30) is zero, implying that a pair of unit vectors in the two lattices coincide. In this case the nearest-neighbour relation can be obtained by solving a similar problem with rank two matrices in order to find the two other base vectors.

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