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Coincidence-Site Lattices

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Coincidence-site lattices are characterized mathematically, in the general case, by a method that can be applied to a pair of original lattices of any symmetry, either metrically identical or metrically different, does not involve inspection and is readily adaptable to computer calculations. The procedure is illustrated by several numerical examples. The proposed characterization of coincidence-site lattices is based on the theory of derivative lattices and makes extensive use of the concepts of superlattice and sublattice. Appended is a simple procedure for determining the transformation matrices needed to generate superlattices and sublattices of any multiplicity.

Introduction

In recent years field-ion and electron-microscopy studies have shown that, in many materials of metallurgical interest, the two crystals forming a grain boundary are often mutually oriented so that they have a common superlattice which continues without disturbance from one crystal to the other. This superlattice is called *coincidence-site lattice* and the two crystals adjacent to the boundary are said to be in a *coincidence-site relationship or coincidence-site related.* The occurrence and importance of coincidence-site lattices was first pointed out by Kromberg & Wilson (1949) in their study on secondary recrystallization of copper. Since then the concept of coincidence-site lattice has been used in the study of the 'structure' of grain boundaries (Brandon, Ralph, Ranganathan & Wald, 1964; Brandon, 1966; Morgan & Ralph, 1967) and in connection with such subjects as grain-boundary migration in high-purity materials (Aust & Rutter, 1959) and nucleation and growth of boundary precipitates (Unwin & Nicholson, 1969).

The interpretation of experimental results in terms of the coincidence-site lattice model requires the knowledge of the geometrical conditions under which two crystals are coincidence-site related. The problem of characterizing mathematically two identical lattices of any symmetry and randomly oriented with respect to each other has been treated by Goux (1961) and Lange (1967). Ranganathan (1966) has given a method for determining the axis and the angle of the rotation necessary to bring two identical cubic lattices, initially coincident, into a coincidence-site relationship and Ranganathan (1967) and Acton & Bevis (1971) have presented comprehensive tables of the angle–axis pairs for the cubic system. The proposed procedure involves several stages of inspection and can only be applied to cubic crystals of the same species.

The mathematical characterization of a coincidence-site lattice of any symmetry and for lattices differing metrically as well as in orientation, may be useful in the analysis of a great variety of grain boundaries and in the study of regular aggregates such as twins and epitaxic and syntaxic intergrowths. As part of a systematic study of the geometrical properties of lattices, a method for the determination of coincidence-site lattices in the general case has been derived. It is essentially an application of the theory of derivative lattices, and its use requires the systematic derivation of superlattices and sublattices of any multiplicity. This derivation can be made either by means of the procedure proposed by Santoro & Mighell (1972) or, more simply, by means of the method presented in the Appendix to this paper.

General

Two lattices Λ' and Λ'' can be coincidence-site related if, and only if, two superlattices, Γ' derived from Λ'

and Γ'' derived from Λ'', are metrically identical. Two lattices which satisfy the above condition are in a coincidence-site relationship if their mutual orientation is such that the superlattices Γ' and Γ'' are coincident. The common superlattice Γ formed by superposing Γ' and Γ'' continues without disturbance from lattice Λ' to lattice Λ'' and is therefore a *coincidence-site lattice*. The characterization of coincidence-site lattices requires the solution of two problems: first, to find the metrically identical superlattices, if any, consistent with the two given original lattices and, second, to specify the mutual orientation of the two lattices when they are coincidence-site related.

Let the lattices Λ' and Λ'' be described by the triplets of primitive translations $\mathbf{a}'_i$ and $\mathbf{a}''_i$, $(i=1,2,3)$ respectively. As there are no restrictions on the choice of $\mathbf{a}'_i$ and $\mathbf{a}''_i$ we will suppose, for simplicity and without loss of generality, that the triplets define the reduced cells of the two lattices (Niggli, 1928; Santoro & Mighell, 1970). The superlattices Γ' and Γ'' can be generated from Λ' and Λ'' by means of the transformations

$$\mathbf{b}'_i=\sum_{j} Q'_{ij}\mathbf{a}'_j \quad (i,j=1,2,3) \tag{1a}$$

and

$$\mathbf{b}''_i=\sum_{j} Q''_{ij}\mathbf{a}''_j . \tag{1b}$$

Methods for evaluating all possible matrices Q generating the unique superlattices for any value of the multiplicity $\Delta=|\mathrm{Q}|$,* and definitions of 'unique' superlattices and sublattices, have been given by Santoro & Mighell (1972; see also Appendix to this paper). The cells based on the translation $\mathbf{b}'_i$ and $\mathbf{b}''_i$ are always considered to be primitive; in general, they are not simply related to the conventional cells† of Γ' and Γ''. For convenience we reduce them by means of the transformations

$$\mathbf{r}'_i=\sum_{j} A'_{ij}\mathbf{b}'_j \tag{2a}$$

and

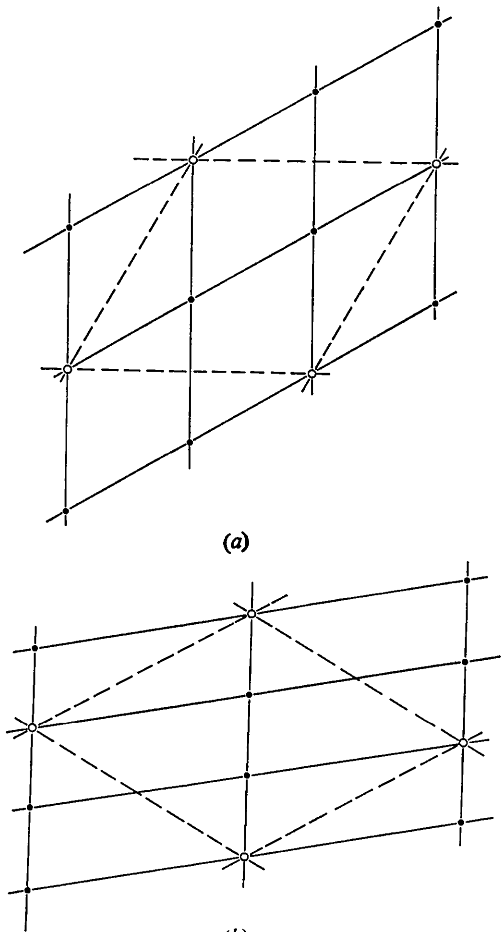
$$\mathbf{r}''_i=\sum_{j} A''_{ij}\mathbf{b}''_j . \tag{2b}$$

Matrices A′ and A″ can be obtained by means of known procedures (Mighell, Santoro & Donnay, 1969). From the above definitions it follows that the lattices Λ' and Λ'' can be in a coincidence-site relationship if, and only if, there are two superlattices Γ' and Γ'' metrically identical, *i.e.* such that we have

$$\mathbf{r}'_i \cdot \mathbf{r}'_j=\mathbf{r}''_i \cdot \mathbf{r}''_j \tag{3}$$

for all values of i and j. To determine if Λ' and Λ'' can be coincidence-site related, we systematically generate, up to any desired multiplicity, all the superlattices of Λ' and Λ'' and check if equation (3) is satisfied. An alternative method is to use the algorithm given by Bucksch (1972) by which the smallest common supercell of two lattices can be found, if any exists, with a minimum of trial and error. Lattices satisfying equation (3) are illustrated in Fig. 1(*a*) and (*b*). In Fig. 2 the two original lattices are shown in a coincidence-site relationship. From this figure, as well as from the definitions previously given, it is evident that the coincidence-site related lattices are sublattices of the coincidence-site lattice.

Let us consider a pair of superlattices Γ' and Γ'' satisfying equation (3). The coincidence-site lattice Γ formed by superposing Γ' and Γ'' can be defined by



(*a*)

(*b*)

Fig. 1. Two original lattices consistent with the same hexagonal primitive superlattice. The reduced form of the superlattice (dashed lines) and those of the original lattice (solid lines) of (*a*) and (*b*) are, respectively,

$$\begin{pmatrix} a_0^2 & a_0^2 & c_0^2 \\ 0 & 0 & -\frac{1}{2}a_0^2 \end{pmatrix} \text{ (hexagonal primitive),}$$

$$\begin{pmatrix} \frac{2}{3}a_0^2 & \frac{2}{3}a_0^2 & c_0^2 \\ 0 & 0 & -\frac{1}{3}a_0^2 \end{pmatrix} \text{ (hexagonal primitive), and}$$

$$\begin{pmatrix} \frac{2}{9}a_0^2 & \frac{14}{9}a_0^2 & c_0^2 \\ 0 & 0 & -\frac{1}{9}a_0^2 \end{pmatrix} \text{ (orthorhombic } C\text{-centered).}$$

The circlets represent nodes common to the superlattice and to the original lattices.

* Δ is also called the 'index' of the vectors $\mathbf{b}_i$ in Λ.

† In this paper we call 'conventional cell' a cell, primitive or centered, whose axes are chosen parallel to symmetry directions of the lattice (*International Tables for X-ray Crystallography*, 1969, p. 6).

either the translations $\mathbf{r}_i'$ or the translations $\mathbf{r}_i''$ of equation (3). If the translations $\mathbf{r}_i'$ are used, then the lattices Λ' and Λ'' are in a coincidence-site relationship if they are sublattices of Γ, *i.e.* if they are related to Γ by the transformations

$$\mathbf{c}_i' = \sum_j P_{ij}' \mathbf{r}_j' \quad (4a)$$

and

$$\mathbf{c}_i'' = \sum_j P_{ij}'' \mathbf{r}_j', \quad (4b)$$

where

$$\mathbf{c}_i' . \mathbf{c}_j' = \mathbf{a}_i' . \mathbf{a}_j' \quad \text{and} \quad \mathbf{c}_i'' . \mathbf{c}_j'' = \mathbf{a}_i'' . \mathbf{a}_j'', \quad (5)$$

and where the matrices P' and P'' represent transformations generating sublattices (Santoro & Mighell, 1972) followed by reduction transformations, as we have assumed that $\mathbf{a}_i'$ and $\mathbf{a}_i''$ define the reduced cells of Λ' and Λ''. In equation (4) the symbols $\mathbf{c}_i'$ and $\mathbf{c}_i''$ are used instead of $\mathbf{a}_i'$ and $\mathbf{a}_i''$ to indicate that the matrices P' and P'' are not necessarily the inverses of $\mathsf{A}'\mathsf{Q}'$ and $\mathsf{A}''\mathsf{Q}''$. From equation (5) it is evident that the multiplicities of the sublattices are $|\mathsf{P}'| = 1/|\mathsf{Q}'|$ and $|\mathsf{P}''| = 1/|\mathsf{Q}''|$.

In general, the cells based on the translations $\mathbf{c}_i'$ and $\mathbf{c}_i''$ have no simple relation to the symmetry elements of the corresponding lattices. Let us perform the transformation

$$\mathbf{e}_i' = \sum_j W_{ij}' \mathbf{c}_j' \quad (6)$$

where the set of translations $\mathbf{e}_i'$ define the conventional cell. Expressions for matrix W' have been tabulated for all possible cases (Mighell, Santoro & Donnay, 1969) or, alternatively, can be evaluated by algebraic means (Bucksch, 1971). If the lattice Λ' possesses symmetry higher than triclinic, then transformation (6) can be expressed in a number of different ways which are symmetrically equivalent. In fact, if M' is one of the symmetry operations of Λ' we have:

$$\mathbf{f}_i' = \sum_j \mathsf{M}_{ij}' \mathbf{e}_j', \quad (7)$$

where the triplets $\mathbf{f}_i'$ and $\mathbf{e}_i'$ are related by the symmetry operation M'. To obtain triplets of the same hand, M' must be restricted to a proper rotation of the lattice. In what follows we will assume $|\mathsf{M}'| = +1$. It is convenient to refer the lattice to a Cartesian system. This is done by means of the transformation

$$\mathbf{y}_i' = \sum_j L_{ij}' \mathbf{f}_j'. \quad (8)$$

The expression of matrix L' depends on how the Cartesian system is attached to the lattice. We take $\mathbf{y}_1'$ coincident with $\mathbf{f}_1'$ and $\mathbf{y}_3'$ coincident with $\mathbf{f}_1' \times \mathbf{f}_2'$ (Busing & Levy, 1967; Santoro, 1970). We set

$$\mathsf{U}' = \mathsf{L}'\mathsf{M}'\mathsf{W}'\mathsf{P}'. \quad (9)$$

The same sequence of transformations involving the lattice Λ'' gives

$$\mathsf{U}'' = \mathsf{L}''\mathsf{M}''\mathsf{W}''\mathsf{P}'', \quad (10)$$

where W'', M'' and L'' are defined as W', M' and L'. If $\mathbf{s}$ is a vector whose components in the reference system $\mathbf{r}_i'$ are the elements of the column vector $\boldsymbol{\sigma}$, then the components of this vector in the systems $\mathbf{y}_i'$ and $\mathbf{y}_i''$ are given by:

$$\mathbf{y}' = (\tilde{\mathsf{U}}')^{-1}\boldsymbol{\sigma}, \quad \mathbf{y}'' = (\tilde{\mathsf{U}}'')^{-1}\boldsymbol{\sigma} \quad (11)$$

where $\tilde{\mathsf{U}}'$ and $\tilde{\mathsf{U}}''$ are the transposes of U' and U'' re-

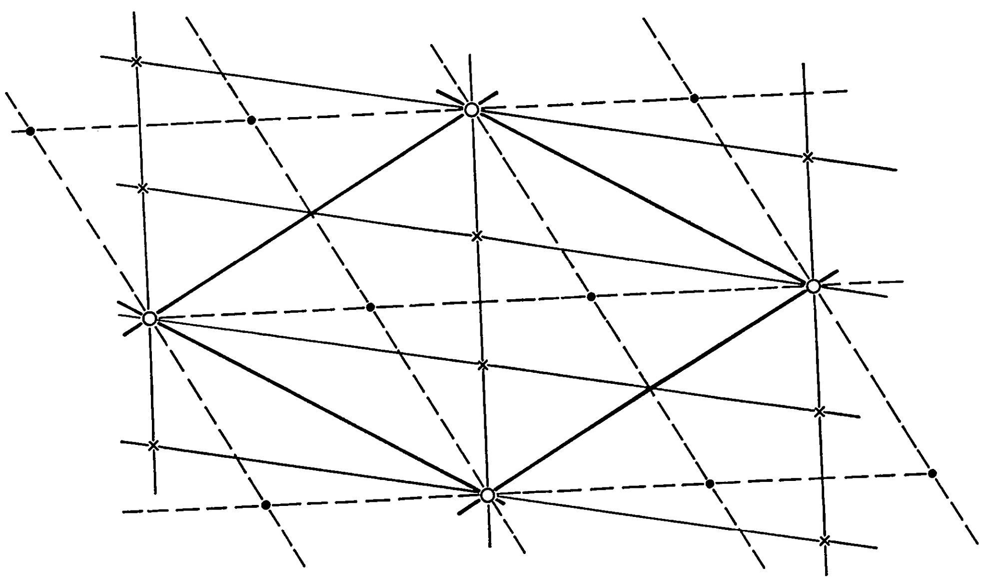


Fig. 2. Lattices of Fig. 1(*a*) and (*b*) mutually oriented so that they are in a coincidence-site relationship. The common superlattice is indicated by heavy lines and the two original lattices by dashed and light lines. The circlets represent nodes common to the superlattice and to both original lattices.

spectively. By solving for $\boldsymbol{\sigma}$ we obtain:

$$\mathbf{y}''=\mathsf{R}\mathbf{y}' \quad (12)$$

where

$$\mathsf{R}=(\tilde{\mathsf{U}}'')^{-1}(\tilde{\mathsf{U}}')=(\tilde{\mathsf{L}}'')^{-1}(\tilde{\mathsf{M}}'')^{-1}\mathsf{D}(\tilde{\mathsf{M}}')\,(\tilde{\mathsf{L}}') \quad (13)$$

and

$$\mathsf{D}=(\tilde{\mathsf{W}}'')^{-1}(\tilde{\mathsf{P}}'')^{-1}(\tilde{\mathsf{P}}')\,(\tilde{\mathsf{W}}')\,. \quad (14)$$

Matrix D defines the coincidence-site relationship of the lattices Λ' and Λ'', *i.e.* the mutual orientation of the two lattices when they are coincidence-site related. The different ways of describing this mutual orientation are obtained from equation (13) by giving M′ and M″ all possible expressions consistent with the symmetry of Λ' and Λ'' respectively.

Special cases

In the general case, the characterization of coincidence-site lattices is carried out first by determining, up to any desired multiplicity Δ, all possible coincidence-site lattices of Λ' and Λ'', *i.e.* all the superlattices that satisfy conditions (3), and second by generating Λ' and Λ'' as sublattices from each possible coincidence-site lattice. In this process all the possible pairs of matrices P′ and P″ necessary for the evaluation of matrix D of equation (14) are determined. Special situations may occur as a consequence of particular geometrical properties of the lattices involved in a coincidence-site relationship. In what follows we will discuss some of the more frequent cases.

It may happen that not all the unique superlattices generated from a given original lattice are metrically different from one another. For example, a cubic primitive lattice of parameter a_0 gives six unique orthorhombic C-centered superlattices of multiplicity $\Delta=3$ having the same reduced cell

$$\begin{pmatrix} a_0^2 & 2a_0^2 & 5a_0^2 \\ -a_0^2 & 0 & 0 \end{pmatrix}. \quad (15)$$

When a group of unique and metrically identical superlattices is generated from either Λ' or Λ'' only one of the group needs to be retained in determining all the possible coincidence-site lattices of Λ' and Λ''.

A case of particular importance in the study of grain-boundary phenomena is encountered when the lattices Λ' and Λ'' are metrically identical. For this special situation the geometrical conditions necessary to have a coincidence-site relationship are always satisfied when $\mathsf{Q}'=\mathsf{Q}''$. This is the same as saying that all the superlattices of Λ' (or Λ'') are possible coincidence-site lattices of Λ' and Λ''. In many cases, however, not all these superlattices give non-trivial coincidence-site relationships. For example, if Λ' and Λ'' are both cubic primitive and metrically identical with parameter a_0, for the multiplicity $\Delta=3$ we have three possible coincidence-site lattices having reduced cells:

$$\begin{pmatrix} a_0^2 & a_0^2 & 9a_0^2 \\ 0 & 0 & 0 \end{pmatrix} (a); \qquad \begin{pmatrix} a_0^2 & 2a_0^2 & 5a_0^2 \\ -a_0^2 & 0 & 0 \end{pmatrix} (b);$$
$$\begin{pmatrix} 2a_0^2 & 2a_0^2 & 3a_0^2 \\ 0 & 0 & -a_0^2 \end{pmatrix} (c)\,. \quad (16)$$

If we generate all the sublattices for $\Delta=\frac{1}{3}$ consistent with the first two superlattices, we obtain the original cubic lattice only once in each case. This result can be interpreted by saying that the matrices P′ and P″ of equation (4a) and (4b) are equal and, consequently, the coincidence-site relationship is trivial. Geometrically, this means that the lattices Λ' and Λ'' are coincident when they are coincidence-site related. On the other hand, if we generate the sublattices of multiplicity $\Delta=\frac{1}{3}$ from the third superlattice, a non-trivial solution results as we find that the original cubic lattice is produced by the following two transformation matrices:

$$\mathsf{P}'=(\tfrac{1}{3}\,\tfrac{\bar{1}}{3}\,\tfrac{\bar{1}}{3}/\tfrac{1}{3}\,\tfrac{2}{3}\,\tfrac{\bar{1}}{3}/\tfrac{2}{3}\,\tfrac{1}{3}\,\tfrac{1}{3}); \quad \mathsf{P}''=(\tfrac{\bar{1}}{3}\,\tfrac{\bar{2}}{3}\,\tfrac{\bar{1}}{3}/\tfrac{\bar{2}}{3}\,\tfrac{\bar{1}}{3}\,\tfrac{1}{3}/\tfrac{\bar{1}}{3}\,\tfrac{1}{3}\,\tfrac{\bar{1}}{3})\,. \quad (17)$$

By noting that reduced and conventional cells are the same for a cubic primitive lattice (W′ = W″ = I, where I is the identity matrix) and that $(\tilde{\mathsf{L}}'')^{-1}=a_0$ and $(\tilde{\mathsf{L}}')=1/a_0$, the expression for matrix R becomes:

$$\mathsf{R}=(\tilde{\mathsf{M}}'')^{-1}(\tilde{\mathsf{P}}'')^{-1}(\tilde{\mathsf{P}}')\,(\tilde{\mathsf{M}}')=$$
$$(\tilde{\mathsf{M}}'')^{-1}(\tfrac{2}{3}\,\tfrac{\bar{1}}{3}\,\tfrac{\bar{2}}{3}/\tfrac{\bar{2}}{3}\,\tfrac{\bar{2}}{3}\,\tfrac{\bar{1}}{3}/\tfrac{\bar{1}}{3}\,\tfrac{2}{3}\,\tfrac{\bar{2}}{3})\,(\tilde{\mathsf{M}}')\,. \quad (18)$$

In certain cases a coincidence-site lattice may be consistent with more than one coincidence-site relationship, *i.e.* with more than one mutual orientation of Λ' and Λ''. This situation arises when two or more of the sublattices generated by means of equation (4a) and/or two or more of the sublattices generated by means of equation (4b) are metrically identical. Let us call P_1', P_2', ... and P_1'', P_2'', ... the matrices generating the sublattice ${}_1\mathbf{c}_i'$, ${}_2\mathbf{c}_i'$, ... and ${}_1\mathbf{c}_i''$, ${}_2\mathbf{c}_i''$, ... respectively, and let us assume

$${}_1\mathbf{c}_i'\,.\,{}_1\mathbf{c}_j'={}_2\mathbf{c}_i'\,.\,{}_2\mathbf{c}_j'=\ldots=\mathbf{a}_i'\,.\,\mathbf{a}_j'$$

and

$${}_1\mathbf{c}_i''\,.\,{}_1\mathbf{c}_j''={}_2\mathbf{c}_i''\,.\,{}_2\mathbf{c}_j''=\ldots=\mathbf{a}_i''\,.\,\mathbf{a}_j''.$$

For each pair of matrices P_m' and P_n'' we calculate a matrix D_{mn} defining a particular coincidence-site relationship of the lattices Λ' and Λ''. Two cases are possible. Let us consider two matrices D_{ab} and D_{cd}. From equation (13) it is evident that, if these matrices are related by any one of the equations

$$\mathsf{D}_{ab}=(\tilde{\mathsf{N}}'')^{-1}\mathsf{D}_{cd}\,, \quad \mathsf{D}_{ab}=\mathsf{D}_{cd}(\tilde{\mathsf{N}}')\,,$$
$$\mathsf{D}_{ab}=(\tilde{\mathsf{N}}'')^{-1}\mathsf{D}_{bc}(\tilde{\mathsf{N}}')\,, \quad (19)$$

where N′ and N″ are symmetry operations of Λ' and Λ'' respectively, then the mutual orientation of Λ' and Λ'' corresponding to D_{ab} and D_{cd} is the same, *i.e.* we have the same coincidence-site relationship. However, if none of equations (19) is satisfied, matrices D_{ab} and D_{cd} define two different mutual orientations of Λ' and Λ'' consistent with the same coincidence-site lattice.

As a first example, let us consider two metrically identical, orthorhombic primitive lattices Λ' and Λ'' of reduced cell

$$\begin{pmatrix} a_0^2/4 & 3a_0^2/4 & c_0^2 \\ 0 & 0 & 0 \end{pmatrix}, \tag{20}$$

where a_0 and c_0 are any suitable parameters. A possible coincidence-site lattice for $\Delta=2$ is hexagonal primitive of reduced cell

$$\begin{pmatrix} a_0^2 & a_0^2 & c_0^2 \\ 0 & 0 & -a_0^2/2 \end{pmatrix}. \tag{21}$$

From this superlattice one obtains three unique sublattices of reduced cell (20) by applying the following transformation matrices:

$$\mathsf{P}_1=(\tfrac{1}{2}00/\tfrac{1}{2}10/001);\quad \mathsf{P}_2=(0\tfrac{1}{2}0/1\tfrac{1}{2}0/00\bar{1});$$
$$\mathsf{P}_3=(\tfrac{1}{2}\,\tfrac{1}{2}0/\tfrac{1}{2}\,\bar{\tfrac{1}{2}}0/00\bar{1}).$$

In this case $\mathsf{W}'=\mathsf{W}''=\mathsf{I}$, so that we obtain:

$$\mathsf{D}_{12}=(\bar{\tfrac{1}{2}}\,\tfrac{3}{2}0/\tfrac{1}{2}\,\tfrac{1}{2}0/00\bar{1});\quad \mathsf{D}_{13}=(\tfrac{1}{2}\,\tfrac{3}{2}0/\tfrac{1}{2}\,\bar{\tfrac{1}{2}}0/00\bar{1});$$
$$\mathsf{D}_{23}=(\tfrac{1}{2}\,\bar{\tfrac{3}{2}}0/\tfrac{1}{2}\,\tfrac{1}{2}0/001).$$

$$\mathsf{R}=\begin{pmatrix} [\cos\alpha+u_1^2(1-\cos\alpha)] & [u_1u_2(1-\cos\alpha)+u_3\sin\alpha] & [u_1u_3(1-\cos\alpha)-u_2\sin\alpha] \\ [u_1u_2(1-\cos\alpha)-u_3\sin\alpha] & [\cos\alpha+u_2^2(1-\cos\alpha)] & [u_2u_3(1-\cos\alpha)+u_1\sin\alpha] \\ [u_1u_3(1-\cos\alpha)+u_2\sin\alpha] & [u_2u_3(1-\cos\alpha)-u_1\sin\alpha] & [\cos\alpha+u_3^2(1-\cos\alpha)] \end{pmatrix}. \tag{24}$$

From these expressions we have:

$$\mathsf{D}_{13}=(\bar{1}00/010/00\bar{1})\mathsf{D}_{12}(100/0\bar{1}0/00\bar{1})$$
$$\mathsf{D}_{23}=(\bar{1}00/010/00\bar{1})\mathsf{D}_{12}.$$

The three matrices, therefore, define only one unique coincidence-site relationship of Λ' and Λ''.

As a second example, let us consider two body-centered monoclinic lattices Λ' and Λ'', metrically equal and having reduced cell

$$\begin{pmatrix} 2a_0^2/3 & a_0^2 & 2a_0^2 \\ a_0^2/3 & a_0^2/3 & a_0^2/3 \end{pmatrix}. \tag{22}$$

For $\Delta=3$ a possible coincidence-site lattice is the orthorhombic C-centered lattice of reduced cell

$$\begin{pmatrix} a_0^2 & 2a_0^2 & 5a_0^2 \\ -a_0^2 & 0 & 0 \end{pmatrix}. \tag{23}$$

From this superlattice one obtains three unique sublattices of reduced cell (22) with the transformation matrices:

$$\mathsf{P}_1=(\tfrac{1}{3}0\tfrac{1}{3}/100/\tfrac{1}{3}1\tfrac{1}{3});\quad \mathsf{P}_2=(\tfrac{1}{3}0\bar{\tfrac{1}{3}}/100/\tfrac{1}{3}\bar{1}\bar{\tfrac{1}{3}});$$
$$\mathsf{P}_3=(\bar{\tfrac{1}{3}}\,\tfrac{1}{3}\,\tfrac{1}{3}/\bar{1}00/\bar{\tfrac{1}{3}}\,\bar{\tfrac{2}{3}}\,\tfrac{1}{3}).$$

For a lattice of reduced cell (22) we have (*International Tables for X-ray Crystallography*, 1969) $\mathsf{W}'=\mathsf{W}''=(0\bar{1}1/\bar{1}00/1\bar{1}\bar{1})$ and, from equation (14), we obtain:

$$\mathsf{D}_{12}=(\bar{\tfrac{1}{3}}\,\tfrac{1}{3}1/\tfrac{2}{3}\,\bar{\tfrac{2}{3}}1/\tfrac{2}{3}\,\tfrac{1}{3}0);\quad \mathsf{D}_{13}=(\bar{\tfrac{1}{2}}\,\bar{\tfrac{1}{2}}0/\bar{\tfrac{3}{2}}\,\tfrac{1}{2}0/\tfrac{1}{6}\,\bar{\tfrac{1}{6}}\bar{1});$$
$$\mathsf{D}_{23}=(\bar{\tfrac{1}{6}}\,\tfrac{1}{6}\bar{1}/\tfrac{5}{6}\,\bar{\tfrac{5}{6}}\bar{1}/\bar{\tfrac{1}{2}}\,\bar{\tfrac{1}{6}}0).$$

These matrices do not satisfy any of equations (19) and, therefore, describe three different coincidence-site relationships, all consistent with the same coincidence-site lattice of reduced cell (23).

Angle–axis pairs

Matrix R of equation (13) expresses the mutual orientation of the coincidence-site-related lattices Λ' and Λ''. This misorientation can also be specified by giving the axis and the angle of the rotation necessary to bring into a coincidence-site relationship the two lattices initially oriented with the reference systems $\mathbf{y}_i'$ and $\mathbf{y}_i''$ coincident. For $\mathsf{L}'=\mathsf{L}''$, *i.e.* if the lattices Λ' and Λ'' are metrically identical and if they are related in the same way to their respective Cartesian systems, the coincidence of $\mathbf{y}_i'$ and $\mathbf{y}_i''$ also means coincidence of the two lattices. If Λ' and Λ'' are not metrically equal, the orientation for which the two Cartesian systems are coincident merely fixes an origin for the relative rotation of the two lattices. By expressing matrix R in terms of the direction cosines u_i of the rotation axis and the rotation angle α about this axis (*International Tables for X-ray Crystallography*, 1959), we obtain:

From this expression we obtain

$$\cos\alpha=(R_{11}+R_{22}+R_{33}-1)/2 \tag{25}$$

and

$$u_1:u_2:u_3=(R_{23}-R_{32}):(R_{31}-R_{13}):(R_{12}-R_{21}). \tag{26}$$

Equations (25) and (26) have been used by Hornstra (1960) in the study of high-angle boundaries in diamond. For $\alpha=180°$ equation (26) becomes indeterminate. In this case we derive, from the expression (24) of matrix R,

$$u_1:u_2:u_3=(R_{11}+1)^{1/2}:(R_{22}+1)^{1/2}:(R_{33}+1)^{1/2}. \tag{27}$$

The relative signs of u_1, u_2 and u_3 can be determined from the signs of R_{12}, R_{13} and R_{23}, through the relations $R_{12}=2u_1u_2$, $R_{13}=2u_1u_3$ and $R_{23}=2u_2u_3$ for $\alpha=180°$.

The direction cosines obtained from (26) and (27) are expressed in the system $(\mathbf{y}_i')$. This system may not be convenient to describe coincidence-site-related lattices in certain cases. It may be useful, therefore, to transform $\mathbf{u}$, the column vector formed by the coordinates u_i, into a more appropriate reference system. For example, the transformation into the system $\mathbf{e}_i'$ defining the conventional cell is

$$\mathbf{v}=\mathsf{T}\mathbf{u}, \tag{28}$$

where

$$\mathsf{T}=\tilde{\mathsf{M}}'\tilde{\mathsf{L}}'. \tag{29}$$

By giving, to M' and M'' of equation (13), the expressions consistent with the proper symmetry operations of the lattices Λ' and Λ'', one obtains all the possible angle–axis pairs relating the two lattices when they are in a coincidence-site relationship. In many cases all the unique angle–axis pairs can be obtained from the simplified equation

$$\mathsf{R}=(\tilde{\mathsf{L}}'')^{-1}(\tilde{\mathsf{M}}'')^{-1}\mathsf{D}(\tilde{\mathsf{L}}')\,, \tag{30}$$

in which M″ must assume all expressions consistent with the symmetry of Λ''. These cases are encountered: (i) when Λ' and Λ'' are both hexagonal or both rhombohedral, or when Λ'' is hexagonal and Λ' rhombohedral; (ii) when neither Λ' nor Λ'' is hexagonal or rhombohedral and Λ' has a symmetry equal to or lower than that of Λ''. If one of the two lattices, say Λ', is hexagonal or rhombohedral, two cases arise: (i) if Λ'' is cubic, tetragonal, or orthorhombic, all the possible angle–axis pairs are obtained from equation (13) in which M″ is given all expressions consistent with the symmetry of Λ'' and M′ is each of the following matrices: $100/010/001$; $010/\bar{1}\bar{1}0/001$; $\bar{1}\bar{1}0/010/00\bar{1}$. (ii) If Λ'' is monoclinic the expressions for M′ must include $100/\bar{1}\bar{1}0/00\bar{1}$; $\bar{1}\bar{1}0/100/001$; $010/100/00\bar{1}$ in addition to the previous ones.

As an example of the application of equations (25), (26) and (27) let us consider the case of two cubic primitive lattices Λ' and Λ'', metrically identical, and having lattice parameter a_0. A possible coincidence-site lattice for $\Delta=3$ is a hexagonal primitive superlattice of reduced cell (16*c*). When Λ' and Λ'' are coincidence-site related, their mutual orientation is expressed by equation (18). As the original lattices are cubic, all the unique angle–axis pairs can be obtained by setting M′ = I. We have, therefore,

$$\mathsf{R}=(\tilde{\mathsf{M}}'')^{-1}(\tfrac{2}{3}\,\tfrac{\bar{1}}{3}\,\tfrac{\bar{2}}{3}/\tfrac{\bar{2}}{3}\,\tfrac{\bar{2}}{3}\,\tfrac{\bar{1}}{3}/\tfrac{\bar{1}}{3}\,\tfrac{2}{3}\,\tfrac{\bar{2}}{3})\,. \tag{31}$$

For M″ = I we obtain, from (25) and (26),

$$\cos\alpha=\frac{\tfrac{2}{3}-\tfrac{2}{3}-\tfrac{2}{3}-1}{2}=-\tfrac{5}{6}\,,\quad \alpha=146{\cdot}4^\circ$$

and

$$R_{23}-R_{32}=-1\,,\quad R_{31}-R_{13}=\tfrac{1}{3}\,,\quad R_{12}-R_{21}=\tfrac{1}{3}\,,$$

i.e. $[u_1u_2u_3]=[\bar{3}11]$. By setting

$$\mathsf{T}=(1/a_0)\,(\bar{1}00/001/010)\,,$$

we have

$$\begin{pmatrix}v_1\\v_2\\v_3\end{pmatrix}=\begin{pmatrix}\bar{1}&0&0\\0&0&1\\0&1&0\end{pmatrix}\begin{pmatrix}\bar{3}\\1\\1\end{pmatrix}=\begin{pmatrix}3\\1\\1\end{pmatrix}.$$

By substituting for M″ the other 23 proper symmetry operations of the cubic lattice, we obtain the following unique angle–axis pairs: [111], $\alpha=60^\circ$, $\alpha'=180^\circ$; [211], $\alpha=180^\circ$; [110], $\alpha=70{\cdot}5^\circ$, $\alpha'=109{\cdot}5$; [210], $\alpha=131{\cdot}8^\circ$; [311], $\alpha=146{\cdot}4^\circ$. These results are in agreement with the angle–axis pairs obtained by other methods. (Acton & Bevis, 1971).

APPENDIX

In a previous paper (Santoro & Mighell, 1972) superlattices and sublattices were defined, and a method for determining the transformation matrices generating the unique superlattices consistent with any given original lattice was presented. This method becomes laborious for large values of the multiplicity of the superlattice. In some crystallographic applications, such as coincidence-site lattice theory, superlattices of high multiplicity play an important role and therefore a simpler and more direct procedure for generating the unique superlattices would be desirable.

Let us consider the axial transformation

$$\mathbf{t}_i=\sum_j S_{ij}\mathbf{a}_j\,, \tag{32}$$

where the triplet of primitive non-coplanar translations $\mathbf{a}_i$ defines any given original lattice. If the elements S_{ij} of matrix S are integers and if the determinant |S| of the transformation is greater than unity, then the translations $\mathbf{t}_i$, considered primitive, define a superlattice of the original lattice. The multiplicity, Δ, of the superlattice is equal to |S| and expresses the ratio of the volume of a primitive cell of the superlattice to that of a primitive cell of the original lattice.

The superlattice generated by transformation (32) can also be generated by any one of the transformation matrices S′ given by the equation

$$\mathsf{S}'=\mathsf{HSK}\,, \tag{33}$$

where the elements H_{ij} and K_{ij} of matrices H and K are integers and give |H| = |K| = 1. If we assume

$$\mathsf{K}=\mathsf{I}\,, \tag{34}$$

where I is the identity matrix, *i.e.* if we impose the condition that the transformations S and S′ must be applied to the same primitive cell of the original lattice, we have

$$\mathsf{S}'=\mathsf{HS}\,. \tag{35}$$

Equation (35) shows that matrices S and S′ can be transformed into each other by a sequence of row additions, *i.e.* they are row equivalent (as the H_{ij} are integers, the elements of a row of matrix S are added to, or subtracted from, the corresponding elements of another row k times, with k an integer.) From equation (35) we have:

$$\mathsf{S}'\mathsf{S}^{-1}=\mathsf{H}\,. \tag{36}$$

Matrices generating the same superlattice are related by equation (36). On the other hand, two superlattices generated by the matrices S and S′ such that $\mathsf{S}'\mathsf{S}^{-1}$ is not a matrix of determinant unity and composed of integral elements are called 'unique'. Unique superlattices are built by using different nodes of the original lattice and may be metrically different or metrically identical. The generation of superlattices can be made without duplication if each class of matrices related by equation (35) can be represented by a uniquely defined matrix. Geometrically, this is equivalent to selecting one primitive cell of the superlattice as a representative of the infinitely many cells describing the same superlattice.

A matrix representing the class defined by equation (35) can be chosen by noting that any matrix S with integral elements S_{ij} and determinant $|S| \geq 1$ can be transformed, by row additions, into an upper triangular matrix Q which satisfies the conditions

$$0 \leq Q_{ij} < Q_{jj}, \quad \text{with} \quad i<j. \tag{37}$$

This can be easily proved by applying the Euclidean algorithm (Niven & Zuckerman, 1962) to the second and third row of S until $S_{31}=0$, then to the first and second row until $S_{21}=0$ and finally to the second and third row until $S_{32}=0$. At this point the elements of the upper triangular matrix can be made positive with appropriate row additions. For example, matrix $(11\bar{2}/\bar{1}21/221)$ can be transformed into the corresponding Q matrix by means of the following row additions:

$$(11\bar{2}/\bar{1}21/221) \rightarrow (11\bar{2}/\bar{1}21/063) \rightarrow (11\bar{2}/03\bar{1}/063) \rightarrow (11\bar{2}/03\bar{1}/005) \rightarrow (113/034/005).$$

Matrix Q belongs to the class of matrices (35) because it is derived from S by row additions and it is uniquely defined because it is possible to prove that: (i) any given matrix S can be transformed by row additions into one and only one Q matrix and (ii) all row-equivalent matrices defined by equation (35) have the same Q matrix. Generating the unique superlattices of any given multiplicity $\Delta=|Q|$ is, therefore, equivalent to deriving all the different matrices Q having determinant equal to Δ, *i.e.* such that

$$Q_{11}Q_{22}Q_{33}=\Delta. \tag{38}$$

As an example of the derivation of Q matrices, let us consider the case $\Delta=3$. From expression (38) and from conditions (37) we immediately write down the 13 different Q matrices generating the 13 unique superlattices of multiplicity 3:

(300/010/001); (100/030/001); (110/030/001); (120/030/001); (100/010/003); (101/010/003); (102/010/003); (100/011/003); (101/011/003); (102/011/003); (100/012/003); (101/012/003); (102/012/003).

From the above procedure it is possible to show that, if Δ is a prime number, then the number n of unique superlattices of multiplicity Δ is given by

$$n=\Delta(\Delta+1)+1.$$

If $\Delta=\Delta_1\Delta_2$, where Δ_1 and Δ_2 are prime numbers, then n is given by

$$n=[\Delta(\Delta+1)+1]+\Delta_1(\Delta_1+1)+\Delta_2(\Delta_2+1)+\Delta(\Delta_1+\Delta_2) \tag{40}$$

if $\Delta_1 \neq \Delta_2$ and by

$$n=[\Delta(\Delta+1)+1]+\Delta_1[\Delta_1(\Delta_1+1)+1] \tag{41}$$

if $\Delta_1=\Delta_2$. The problem for $\Delta=\Delta_1\Delta_2\Delta_3$, where Δ_1, Δ_2, Δ_3 are primes, is more complex as the Q_{ij}'s may assume any of the following values: $1, \Delta, \Delta_1, \Delta_2, \Delta_3, \Delta_1\Delta_2, \Delta_1\Delta_3, \Delta_2\Delta_3$. Even in this case the Q matrices can readily be derived.

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