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Permissible Angles for Coincidence-Site-Lattice Rotations

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Abstract

In addition to symmetry rotations ($\Sigma = 1$), lattices may admit coincidence-site-lattice (c.s.l.) rotations of various degrees of coincidence, Σ. The conditions for the occurrence of c.s.l. rotations are formulated in general terms by introducing the metric matrix of a lattice. When all lattices are considered, it is found that there are 4Σ possible values for the angle of rotation which give rise to a degree of coincidence Σ. These angles have cosines which are integral multiples of $1/2\Sigma$. A particular lattice admits only some of these c.s.l. rotations. Cubic lattices are discussed in detail and it is shown that the number of permissible rotation angles for each odd value of Σ is approximately $3{\cdot}414 \times \sqrt{\Sigma}$. Conversely, a particular rotation angle originates a c.s.l. of degree of coincidence Σ in those lattices which satisfy particular metric conditions. Finally, the effect of a uniform strain due to temperature or pressure changes is analysed, and it is shown that while symmetry rotations are invariant to this form of strain, only very few c.s.l. rotations are unaffected.

1. Introduction

The symmetry rotations of a space lattice bring it into self-coincidence. These rotations involve one of the angles 60, 90, 120, 180°, and it is usual to classify the space lattices in various systems according to the rotational symmetry they possess. It is convenient to think of two interpenetrating lattices, identical to the lattice under consideration, which are initially in the same orientation and therefore show total coincidence of their lattice points. If one of the lattices is now given a symmetry rotation, total coincidence of lattice points will again occur. In addition to self-coincidence rotations, space lattices may admit partial-coincidence rotations. Upon such a rotation, a fraction $1/\Sigma$ of the lattice points in each of the two interpenetrating lattices comes into coincidence with lattice points of the other lattice. The coincident points define a space lattice – the coincidence-site lattice (c.s.l.). The c.s.l. is a sub-lattice of the original lattice, and Σ is the ratio of the volumes of unit cells in the c.s.l. and in the original lattice. The degree of coincidence Σ is therefore an integer. The c.s.l. orientations for each Σ are likely to occur for a discrete and finite set of rotation angles, in the same way as the symmetry rotations can only occur for one of the four angles indicated above. The main objective of this paper is to derive the permissible angles θ_i for each value of Σ and to formulate the conditions that a lattice must satisfy in order to admit a particular c.s.l. rotation (Σ,θ_i).

Matrix algebra has proved a very convenient method of studying the properties of coincidence-site and related lattices (Warrington & Bufalini, 1971; Fortes, 1972*a*, 1977; Grimmer, Bollmann & Warrington, 1974; Grimmer, 1976). In the present paper we shall extend previous work along this line and show how the c.s.l. theory can be simply formulated in terms of the metric matrix of a lattice. It is within this formulation that we shall solve the problems enunciated above. The advantages of using the metric matrices in the study of c.s.l.'s of two different lattices will be discussed elsewhere.

Attention will also be given in this paper to the effect of strain on the symmetry and c.s.l. rotations of a lattice. When a lattice is strained, its metric is changed; if the strain is due to temperature or pressure changes, symmetry rotations are unaffected, but, except in cubic lattices, only c.s.l. rotations about high-symmetry axes will be preserved.

2. C.s.l. rotation matrices

We take a vector basis ($\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3$) of a lattice and introduce the metric matrix $\mathbf{G} = [(g_{ij})]$ with $g_{ij} = \mathbf{e}_i.\mathbf{e}_j$. The set of vectors $[\hat{\mathbf{e}}_1\,\hat{\mathbf{e}}_2\,\hat{\mathbf{e}}_3] = [\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3]\,\mathbf{T}$, meaning that $\hat{\mathbf{e}}_i = \sum_j t_{ji}\mathbf{e}_j$, with $\mathbf{T} = [(t_{ij})]$, constitutes another basis for the same lattice if $\mathbf{T}$ is an integral matrix with a determinant equal to ± 1 (in which case $\mathbf{T}^{-1}$ is also an integral matrix). The metric matrix in the new basis is $\hat{\mathbf{G}} = \mathbf{T}^T\mathbf{G}\mathbf{T}$, where $\mathbf{T}^T$ is the transpose of $\mathbf{T}$.

A rotation of a space lattice with a basis ($\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3$) is defined by a matrix $\mathbf{R}$ (expressed in that basis) which satisfies the condition (*e.g.* Korn & Korn, 1968)

$$\mathbf{R}^T\mathbf{G}\mathbf{R} = \mathbf{G}. \qquad (1)$$

If the basis is changed (matrix $\mathbf{T}$) the same rotation is represented by $\mathbf{T}^{-1}\mathbf{R}\mathbf{T}$. A matrix $\mathbf{R}$ satisfying equation (1) defines a c.s.l. rotation if and only if $\mathbf{R}$ is rational.

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This result has been widely used in the study of cubic and hexagonal lattices (*e.g.* Grimmer *et al.*, 1974; Warrington, 1976). Recently, Grimmer (1976) has given a formal proof of its general applicability and has also shown that the degree of coincidence is the smallest integer Σ such that both $\Sigma\mathbf{R}$ and $\Sigma\mathbf{R}^{-1}$ are integral matrices. These properties are, of course, independent of the vector basis chosen.

For a given lattice (given $\mathbf{G}$) the c.s.l. rotations are then defined by rational matrices $\mathbf{R}$ which satisfy condition (1). In addition to Σ, it is important to determine, for each $\mathbf{R}$, the axis and the angle of rotation. The axis $\mathbf{v} = \sum_j v_j \mathbf{e}_j$ is obtained from $\mathbf{R}\mathbf{v} = \mathbf{v}$; in this matricial equation $\mathbf{v}$ is the column vector $[(v_j)]$. The vector $\mathbf{v}$ always defines a lattice direction, *i.e.* $\mathbf{v}$ is parallel to a lattice vector (Fortes, 1972*b*). The angle of rotation can be obtained from

$$t = 2\cos\theta + 1, \qquad (2)$$

where t is the trace of $\mathbf{R}$ (*i.e.* the sum of the elements in the diagonal of $\mathbf{R}$). In the following, we shall attach special importance to Σ and θ, and refer to a c.s.l. rotation by indicating its pair (Σ,θ), as is usually done for symmetry rotations. It should be noted that for a particular pair (Σ,θ), a lattice may admit two (and possibly more than two) c.s.l. rotations not symmetrically related (an example is given by Grimmer *et al.*, 1974), and that two or more different pairs (Σ,θ) may be associated with identical c.s.l.'s of a particular lattice. These complications do not affect the following analysis which has the purpose of finding the set of permissible pairs (Σ,θ) for c.s.l. rotations of an arbitrary lattice.

3. Rotation angles for partial coincidence

We now consider the rational matrices of the type $\mathbf{R} = (1/\Sigma)[(n_{ik})]$, where n_{ik} are integers ($i, k = 1, 2, 3$), and Σ is the smallest integer such that both $\Sigma\mathbf{R}$ and $\Sigma\mathbf{R}^{-1}$ are integral matrices. As mentioned above, c.s.l. rotations are expressed by matrices of this type, the degree of coincidence being the integer Σ. The angle of rotation is given by [*cf.* equation (2)]

$$1 + 2\cos\theta = \frac{1}{\Sigma}\sum_i n_{ii}. \qquad (3)$$

The first term can only vary between -1 and 3. Therefore, the integer $\sum_i n_{ii}$ may vary between $-\Sigma$ and 3Σ. If $\sum_i n_{ii}$ can take all the integral values between these limits, then the possible angles for c.s.l. rotations of degree of coincidence Σ will be given by

$$\cos\theta_k = \frac{k-\Sigma}{2\Sigma}$$

$$\text{with } k = -\Sigma, -\Sigma+1, \cdots, 0, \cdots, 3\Sigma - 1. \qquad (4)$$

We have omitted the value $k = 3\Sigma$ which corresponds to $\theta = 0$. With $k - \Sigma = i$, equation (4) can be written as

$$\cos\theta_i = \frac{i}{2\Sigma} \quad \text{with} \quad i = -2\Sigma, \cdots, 0, \cdots, 2\Sigma - 1. \qquad (5)$$

The previous argument is analogous to that used by Bhagavantan (1966) to find the possible angles of symmetry rotations of a space lattice. The argument can be generalized to n-dimensional lattices (the trace of a rotation matrix of rank n is $2\cos\theta + n - 2$) with the result that the possible angles for c.s.l. rotations are still given by equation (5). No more symmetry or c.s.l. rotation angles appear in higher-dimension lattices.

It is now necessary to show that there is at least a lattice for which a rotation of any of the angles θ_i given by equation (5) originates partial coincidence of degree Σ. We shall prove this for the case of three-dimensional lattices. Consider a lattice with a basis $(\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3)$ such that $|\mathbf{e}_2| = \Sigma|\mathbf{e}_1|$ and the angle between $\mathbf{e}_1$ and $\mathbf{e}_2$ is equal to θ_i, with $\cos\theta_i$ given by equation (5); $\mathbf{e}_3$ is perpendicular to both $\mathbf{e}_1$ and $\mathbf{e}_2$. We have

$$\mathbf{G} = \begin{pmatrix} e_1^2 & \frac{i}{2}e_1^2 & 0 \\ \frac{i}{2}e_1^2 & \Sigma^2 e_1^2 & 0 \\ 0 & 0 & e_3^2 \end{pmatrix}.$$

A rotation of angle θ_i about $\mathbf{e}_3$ is expressed by the matrix [*cf.* equations (1) and (2)]

$$\mathbf{R} = \begin{pmatrix} 0 & -\Sigma & 0 \\ 1/\Sigma & i/\Sigma & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The degree of coincidence is therefore Σ for all values of i ($\Sigma\mathbf{R}^{-1}$ is also an integral matrix). We see that for each of the rotation angles given by equation (5) there are lattices which achieve partial coincidence of degree Σ. And there are no more c.s.l. rotations for each Σ than those given by equation (5).

To summarize the results obtained so far in this section, we may conclude that partial coincidence of a given degree Σ can only be achieved for particular angles of rotation (in number 4Σ) of a lattice. The possible angles are given by equation (5); their cosines are the integral multiples of $1/2\Sigma$. Of course, an arbitrary lattice will admit only some of these c.s.l. rotations and frequently none. These results can be regarded as a generalization of the well known properties of symmetry rotations of lattices to include c.s.l. rotations.

Table 1. *Angles of rotation (°) for partial coincidence (c.s.l.)*

Degree of coincidence		
$\Sigma=1$	$\Sigma=2$	$\Sigma=3$
		33·56
	41·41	
		48·19
60·00	60·00	60·00 (*c*)
		70·53 (*c*)
	75·52	
		80·41
90·00 (*c*)*	90·00	90·00
		99·59
	104·48	
		109·47 (*c*)
120·00 (*c*)	120·00	120·00 (*c*)
		131·81 (*c*)
	138·59	
		146·44 (*c*)
180·00 (*c*)	180·00	180·00 (*c*)

* Angles of rotation in a cubic lattice.

The rotations of 180, 120, 90 and 60° are among the possible c.s.l. rotations for all values of Σ. In Table 1 we give the values of the angles of rotation for c.s.l.'s with $\Sigma = 1, 2, 3$ (the values for partial coincidence in a cubic lattice are indicated; *cf.* Warrington & Bufalini, 1971). We note that if θ_i is a possible angle, $(180°-\theta_i)$ is also possible, though not necessarily in the same lattice.

4. Permissible angles for c.s.l. rotations of a particular lattice

In a recent publication (Fortes, 1977) it has been shown that lattices can be classified into various categories, depending on the incidence of c.s.l. rotations they admit. The important category is what are termed C lattices, *i.e.* lattices which admit c.s.l. rotations about any lattice direction. As shown by Fortes (1977), the C lattices are characterized by a metric $\mathbf{G}$ of the type $\mathbf{G} = \lambda \mathbf{I}_0$, where λ is a number (which can be taken equal to 1 by choosing a convenient unit to measure the lattice parameters) and $\mathbf{I}_0$ is an integral matrix. Next to C lattices there are lattices which admit c.s.l. rotations (with $\theta \neq 180°$) about one and only one direction, and lattices which admit only 180° c.s.l. rotations. Finally there are lattices which do not admit any c.s.l. rotations. The matrices $\mathbf{G}$ for each of these three types must conform to certain conditions, which we shall indicate in § 5.

We note that any lattice can be approximated by a C lattice as closely as desired, in the same way that a real number can be approximated by a rational number as closely as desired; therefore, any lattice can be treated, with an accuracy as large as desired, as a C lattice.

In order to find if a particular lattice admits a c.s.l. rotation defined by a given pair (Σ,θ_i), related by equation (5), it is necessary to find whether a rational matrix $\mathbf{R}$ exists, satisfying equation (1), with a trace $t = 2\cos\theta_i + 1$, and such that Σ is the smallest integer for which both $\Sigma\mathbf{R}$ and $\Sigma\mathbf{R}^{-1}$ are integral matrices.

This problem can be solved by first writing the general form of $\mathbf{R}$ in a particular lattice basis, and then, by inspection, finding the pairs (Σ,θ_i) for which both $\Sigma\mathbf{R}$ and $\Sigma\mathbf{R}^{-1}$ are integral matrices. The general form of $\mathbf{R}$ is of the type $\mathbf{T}^{-1}\mathbf{R}_c\mathbf{T}$ where $\mathbf{R}_c$ is an orthogonal matrix (*i.e.* a θ_i rotation matrix in an orthonormal basis, the form of which is well known) and $\mathbf{T}$ is the matrix that relates a vector basis of the lattice to the orthonormal basis (this is not, in general, a lattice basis, and therefore $\mathbf{T}$ is not an integral matrix).

A particularly important case is that of cubic lattices, for which the problem can be completely solved by making use of the well known relations between the angle of rotation and the degree of coincidence (Ranganathan, 1966; Grimmer *et al.*, 1974). The permissible angles θ_i for c.s.l. rotations of a cubic lattice are those for which

$$\operatorname{tg}\theta_i/2 = \frac{x}{y}R, \tag{6}$$

where x and y are coprime integers and $R^2 = \sum_j n_j^2$, n_j being coprime integers (the Miller indices of the rotation axes). Writing

$$C = x^2 + y^2R^2, \tag{7}$$

the degree of coincidence is the odd integer among C, $C/2$ and $C/4$.

Let us now find the number of permissible angles θ_i for each (odd) value of Σ. Since $\cos\theta_i = i/2\Sigma$ we have

$$\operatorname{tg}\frac{\theta_i}{2} = \frac{(4\Sigma^2 - i^2)^{1/2}}{2\Sigma + i}. \tag{8}$$

Writing $2\Sigma + i = p^2/Q$, where $1/Q$ is an integer without a square factor, and inserting this in equation (8) we obtain [from the rule defined in equations (6) and (7)], after eliminating the factor p, a value $C' = 4\Sigma/Q$. This C' may differ from the correct C by a square factor n^2, if n^2 divides both p^2/Q^2 and $(2\Sigma - i)/Q$, *i.e.* $4\Sigma/Q = n^2\alpha\Sigma$ ($\alpha = 1, 2, 4$). If the θ_i rotation of a cubic lattice is to give rise to a degree of coincidence Σ, it is then necessary that $Q = 1$ or $Q = \frac{1}{2}$, which are the only solutions of the previous equation. It follows that the possible angles for a particular odd value of Σ are those for which i satisfies the condition

$$2\Sigma + i = p^2 \quad \text{or} \quad 2q^2 \quad (-2\Sigma \leq i < 2\Sigma), \tag{9}$$

p and q being integers (we take $p \geq 1$ and $q \geq 0$). In addition, it is necessary that $(1/Q)(2\Sigma - i)$ be different from a u number, *i.e.* an integral number which cannot be written as the sum of three squares. The u numbers

(7, 15, 23, 28, 31,...) are all one of the types $8n-1$ or $4m$ (n, m are positive integers). It is then easy to see that the condition $(1/Q)(2\Sigma - i) \neq u$ number is always satisfied for $2\Sigma + i = 2q^2$, but not for $2\Sigma + i = p^2$. For a given Σ the number, b, of these forbidden cases is the number of ways in which Σ can be written as the sum of a square (1, 4, 9,...) plus a u number. The incidence of these special cases is small: b is at most one for $\Sigma < 43$, at most two for $\Sigma < 107$, *etc.*

The number of permissible values of i for each Σ is easily found [see equation (9)]:

$$I(4\Sigma - 1)^{1/2} + I\left(\frac{4\Sigma - 1}{2}\right)^{1/2} + 1 - b, \qquad (10)$$

where $I(x)$ is the largest integer not greater than x. This sum is approximately

$$I\left[\left(1 + \frac{1}{2^{1/2}}\right)(4\Sigma)^{1/2}\right] - b, \qquad (11)$$

and since b is small compared with the other term, we may conclude that the number of different rotation angles of a cubic lattice giving rise to a c.s.l. of degree of coincidence Σ (Σ odd) is approximately the closest integer to $3{\cdot}414\Sigma^{1/2}$. This figure should be compared with that, 4Σ, valid for the totality of lattices.

5. The occurrence of a particular c.s.l. rotation

The inverse problem to that discussed in the previous section is to determine the lattices (or, equivalently, the metric matrices $\mathbf{G}$) which admit a c.s.l. rotation defined by a particular pair (Σ,θ) related by equation (5). This problem can be formally solved by imposing the same conditions on the rotation matrix. Before delineating a detailed solution, we note that multiplication of the basic vectors by the same real number μ (so that $\mathbf{G}$ is multiplied by μ^2) does not affect the c.s.l. rotations; and if a c.s.l. rotation (Σ,θ_i) exists in a lattice, it also exists in the reciprocal lattice (metric matrix $\mathbf{G}^{-1}$), the rotation matrix being $(\mathbf{R}^{-1})^T$ in the reciprocal basis. This last property shows that two lattices in a reciprocal relationship admit the same c.s.l. rotations and, in particular, have the same symmetry.

Let us now show how it is possible to find the metric of the lattices which admit a particular $[\Sigma,\theta = \cos^{-1}(i/2\Sigma)]$ c.s.l. rotation. In all such lattices the axis for this rotation is necessarily parallel to a lattice vector $\mathbf{e}_1$, which is perpendicular to a lattice plane Π (Fortes, 1972*b*). One can always take a vector basis $(\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3)$ of these lattices with one of the vectors $(\mathbf{e}_1)$ parallel to the rotation axis, and another $(\mathbf{e}_2)$ in the lattice plane Π and therefore normal to $\mathbf{e}_1$. To simplify we make $|\mathbf{e}_1| = 1$. Consider now a set of orthonormal vectors $(\mathbf{c}_1\,\mathbf{c}_2\,\mathbf{c}_3)$ with $\mathbf{c}_1 = \mathbf{e}_1$ and $\mathbf{c}_2$ parallel to $\mathbf{e}_2$. The matrix $\mathbf{C}$ in $[\mathbf{c}_1\,\mathbf{c}_2\,\mathbf{c}_3] = [\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3]\mathbf{C}$ can be written in the form:

$$\mathbf{C} = \begin{pmatrix} 1 & 0 & k_1 \\ 0 & 1/\lambda & k_2 \\ 0 & 0 & k_3 \end{pmatrix}.$$

The metric matrix of the lattice, referred to the basis $(\mathbf{e}_1\,\mathbf{e}_2\,\mathbf{e}_3)$, is $\mathbf{G} = (\mathbf{C}\mathbf{C}^T)^{-1}$. The lattice is now rotated by θ about $\mathbf{e}_1$. The rotation matrix is

$$\mathbf{R}_c = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}$$

in the orthonormal basis, and $\mathbf{R} = \mathbf{C}\mathbf{R}_c\,\mathbf{C}^{-1}$ in the lattice basis.

Writing $a_j = \lambda k_j \sin\theta$ ($j = 1, 2, 3$) and $\cos\theta = i/2\Sigma$ we obtain for the matrices $\Sigma\mathbf{R}$ and $\Sigma\mathbf{R}^{-1}$ the expression

$$\Sigma\mathbf{R}^{\pm 1} = \begin{pmatrix} \Sigma & \pm a_1\Sigma & \dfrac{a_1\Sigma}{a_3}\left(-1 + \dfrac{i}{2\Sigma} \mp a_2\right) \\ 0 & \dfrac{i}{2} \pm a_2\Sigma & \mp\left(\dfrac{a_2^2\Sigma}{a_3} + \dfrac{4\Sigma^2 - i^2}{4\Sigma a_3}\right) \\ 0 & \pm\Sigma a_3 & \mp\Sigma a_2 + \dfrac{i}{2}\ , \end{pmatrix} \qquad (12)$$

and for the metric matrix

$$\mathbf{G} = \begin{pmatrix} 1 & 0 & -\dfrac{a_1}{a_3} \\ 0 & \lambda^2 & -\dfrac{a_2}{a_3}\lambda^2 \\ -\dfrac{a_1}{a_3} & -\dfrac{a_2}{a_3}\lambda^2 & \left(\dfrac{a_1}{a_3}\right)^2 + \lambda^2\left(\dfrac{a_2}{a_3}\right)^2 + \dfrac{\lambda^2}{a_3^2}\left(\dfrac{4\Sigma^2 - i^2}{4\Sigma^2}\right) \end{pmatrix}. \qquad (13)$$

When $\theta = 180°$ ($i = -2\Sigma$) these expressions still apply if we make $a_i = 0$, $(4\Sigma^2 - i^2)/a_3 = 0$, and assume that a_1/a_3, a_2/a_3 remain finite.

The lattices that admit the particular c.s.l. rotation $[\Sigma, \theta = \cos^{-1}(i/2\Sigma)]$ are those defined by metric matrices of the type $\mu^2 \mathbf{G}$, where μ is any real number, and $\mathbf{G}$ is given by equation (13), and where λ is another real number and a_1, a_2, a_3 are numbers such that the elements in the matrices $\Sigma\mathbf{R}^{\pm 1}$ [equation (12)] are integers without a common divisor.

For $\theta \neq 180°$, the numbers a_1, a_2, a_3 are necessarily rational. Finding the a_i's is, in general, a somewhat tricky problem in the field of integral numbers. In this case, if λ^2 is also rational the lattices defined by $\mathbf{G}$ are C lattices; if λ^2 is not rational the lattices admit only c.s.l. rotations (with $\theta \neq 180°$) about $\mathbf{e}_1$. Finally, a 180° c.s.l. rotation of degree of coincidence Σ occurs provided a_1/a_3 is a rational number such that $2\Sigma(a_1/a_3)$ is an integer coprime with Σ. The metric matrix $\mathbf{G}$ is then of the form

$$\mathbf{G} = \begin{pmatrix} 1 & 0 & -a_1/a_3 \\ 0 & \lambda^2 & \varphi \\ -a_1/a_3 & \varphi & \psi^2 \end{pmatrix}, \qquad (14)$$

where λ, φ, ψ are any real numbers (with the only restriction that $\mathbf{G}$ is a metric matrix).

In all cases the basis $(\mathbf{e}_1\, \mathbf{e}_2\, \mathbf{e}_3)$ can be transformed by an integral matrix $\mathbf{T}$ (with det $\mathbf{T} = \pm 1$) into a more convenient basis ($\mathbf{G}$ is transformed into $\mathbf{T}^T\mathbf{G}\mathbf{T}$) – for example, one that shows the Bravais type of lattice. For example, if the matrix $\mathbf{G}$ [equations (13) or (14)] can be transformed into a unit matrix, the lattice defined by $\mathbf{G}$ is a simple cubic lattice.

6. Effect of strain on c.s.l. rotations

When a lattice is uniformly strained its vector basis is altered. We introduce the matrix $\mathbf{S} = [(s_{ij})]$ which relates crystallographically equivalent bases in the unstrained and strained lattices. More precisely, $\mathbf{S}$ is chosen such that, for small strains, $s_{ij} \simeq 1$ and $s_{ij} \simeq 0$. Since the metric is changed, symmetry and c.s.l. rotations will, in general, be affected. Consider two identical interpenetrating lattices in a c.s.l. orientation. In general, the strain will affect the two lattices differently and in the strained 'bicrystal' the two lattices are no longer identical. This is the relevant situation in the case of elastically anisotropic crystals deformed by a uniform stress. Its analysis, from the point of view of the c.s.l. relations, can be made using Grimmer's (1976) method for the study of c.s.l.'s between different lattices.

We shall consider only the strain due to a scalar stimulus (*e.g.* temperature and pressure changes). In such cases, the two strained lattices are still identical. If their relative orientation in the unstrained condition is defined by a rotation matrix $\mathbf{R}$ (axis of misorientation $\mathbf{v}$, angle of rotation θ), then the relative orientation in the strained condition is defined by $\mathbf{S}^{-1}\mathbf{R}\mathbf{S}$, and while θ is unchanged, the new axis of rotation, $\mathbf{S}\mathbf{v}$, will not in general be crystallographically equivalent to the original axis. The matrix $\mathbf{S}$ can be obtained from the thermal expansion or elastic properties of the crystal, depending on the strain stimulus [see, for instance, Bhagavantan (1966)]. For example, in orthorhombic crystals the matrix $\mathbf{S}$ relating vector bases parallel to the orthorhombic axes is a diagonal matrix, no two diagonal elements being equal.

Suppose that $\mathbf{R}$ is a rational matrix which defines a c.s.l. rotation of the unstrained lattice. Then $\mathbf{S}^{-1}\mathbf{R}\mathbf{S}$ will not, in general, be rational and therefore does not define a c.s.l. rotation. There are, however, some important exceptions to this situation, which can be found from a consideration of the form of $\mathbf{S}$ in the various symmetry systems. The invariant cases, *i.e.* c.s.l. orientations which are not destroyed by thermal or hydrostatic pressure strains, are the following: (1) all symmetry rotations; (2) all c.s.l. rotations in cubic lattices; (3) all c.s.l. rotations about threefold (*i.e.* trigonal), fourfold (*i.e.* tetragonal) and sixfold (*i.e.* hexagonal) axes of symmetry.

It should be noted that even 180° c.s.l. rotations are, in general, affected, although coincidence in the lattice plane perpendicular to the rotation axis (*i.e.* the twin plane) is not destroyed.

Finally, we would like to draw attention to the possibility that these effects of strain (particularly stress-induced strain) in the distribution of atomic sites at a grain boundary may give rise to significant (and possibly irreversible) changes in the boundary atomic structure, especially in the case of c.s.l. or near c.s.l. boundaries. It should be interesting to analyse the possibility of these changes being accomplished by the emission or absorption of point or line defects at the boundary.

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