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The Double Shear Geometry and Associated Rational Orientational Relationships

LARA BERAHA AND MICHEL DUNEAU

Centre de Physique Théorique, CNRS UPR A0014, Ecole Polytechnique, 91128 Palaiseau CEDEX, France

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Abstract

The orientational relationships between two lattices of equal density can be analysed by the factorization of their transition matrices into a product of no more than four shears with rational directions. The particular cases where a coincidence lattice exists correspond to a factorization into at most two completely rational shears. The present paper gives a geometrical analysis of these situations. The main result is a classification that is different from the usual one in terms of the coincidence index Σ. The relationship between these two approaches is given in detail and some experimentally observed examples are discussed.

1. Introduction

The aim of mathematical crystallography is the classification of periodic structures by means of different equivalence relationships, yielding the well known crystallographic classes and Bravais lattices. Crystallography is based on an analysis of the symmetry operations associated with these structures. Such operations are the isometric transformations that leave the structure unchanged, *i.e.* that bring the transformed structure into full coincidence with the original one. In this respect, the most important generalization of this analysis is the consideration of particular symmetries for which the initial and the transformed structure only partially coincide on a common sublattice. This new development of crystallography was initiated by Bollmann (1970, 1982), who introduced the notions of coincidence site lattices (CSL), displacement shift complete lattices (DSC) and O lattices. This approach has received growing interest both from theorists and experimentalists, particularly in the field of interfaces and grain boundaries (see, for instance, Pond 1989). Furthermore, the notion of a CSL was recently extended in the case of quasiperiodic structures with non-crystallographic symmetries by Warrington & Radulescu (1995).

In this paper, we propose a new analysis of coincidence lattices and related orientation relationships. This analysis is based on the properties of the transition matrix between two lattices: If L_a and L_b are lattices with bases $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ and $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$, the corresponding transition matrix T is defined by $\mathbf{b}_i = \sum T_{ji}\mathbf{a}_j$. Now, if T has determinant 1, there exists a factorization of T as a product of at most *four* shear matrices with rational shear directions (Duneau & Oguey, 1991; Duneau, 1992). These shear transformations are of the form $S = I + |\mathbf{s}\rangle\langle\boldsymbol{\sigma}|$, where $\mathbf{s}$ is an irreducible vector with integer entries and $\boldsymbol{\sigma}$ is a covector orthogonal to $\mathbf{s}$. Since $S\mathbf{x} = \mathbf{x} + \langle\boldsymbol{\sigma}, \mathbf{x}\rangle\mathbf{s}$, the vector $\mathbf{s}$ defines the shear direction and the covector $\boldsymbol{\sigma}$ specifies the invariant plane. The point is that for particular pairs of lattices and for particular relative orientations, the transition matrix T may be factorized into less than four shear matrices: the number of shears required to map L_a onto RL_b is a function of the rotation R. For instance, if there are two reciprocal vectors $\mathbf{q}_a \in L_a^*$ and $\mathbf{q}_b \in L_n^*$ (L^* denotes the reciprocal lattice of L) having the same length, *i.e.* $|\mathbf{q}_a| = |\mathbf{q}_b|$ and if R is any rotation such that $\mathbf{q}_a = R\mathbf{q}_b$, the transition matrix T between L_a and RL_b can be factorized into at most *three* shears. Within this class of rotations, there are particular ones, for which at most *two* shears are required for the factorization. For these situations, there exists an intermediate lattice which is a simple shear deformation of both L_a and RL_b. These particular orientational relationships are believed to have physical relevance and will be considered in this paper. A similar approach was used in Donnadieu & Duneau (1994) to give a new analysis of orientational relationships in some duplex steels. Moreover, it was proved by Duneau, Oguey & Thalal (1992) that whenever L_a and RL_b share a coincidence lattice the double shear condition is satisfied with the further property that the shear matrices have rational entries. The main purpose of this paper is to give a simple method to compute and to identify these cases.

In §2, we recall standard properties of shear transformations. In §3.1, we consider the double shear condition and give a simple method to identify the corresponding orientational relationships. In §3.2, we treat the example of rotations of cubic lattices, which are associated with a coincidence site lattice. In §4, we show how one can determine the shear transformation corresponding to a given rotation axis $\mathbf{q}$, a rotation angle φ and a given index Σ of the CSL. In the last section, we will compare experimental observations of mechanical twins in silicon obtained by Putaux & Thibault-Dessaux (1990) with our theoretical calculations of some measured quantities.

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2. Shear transformations and fractional shears

For completeness, we recall some useful properties of shear transformations (Duneau & Oguey, 1991; Duneau, 1992). By definition, a 3D shear transformation is a linear mapping which reads:

$$S = I + |\mathbf{s}\rangle\langle\boldsymbol{\sigma}| = \begin{bmatrix} 1+s_1\sigma_1 & s_1\sigma_2 & s_1\sigma_3 \\ s_2\sigma_1 & 1+s_2\sigma_2 & s_2\sigma_3 \\ s_3\sigma_1 & s_3\sigma_2 & 1+s_3\sigma_3 \end{bmatrix} \tag{1}$$

so that its action is given by

$$S(\mathbf{x}) = \mathbf{x} + \langle\boldsymbol{\sigma}, \mathbf{x}\rangle\mathbf{s}, \tag{2}$$

where $\langle\boldsymbol{\sigma}, \mathbf{x}\rangle$ denotes the scalar product between direct space and reciprocal space.

We assume that $\mathbf{s}$ is an irreducible vector of some lattice L (the indices of $\mathbf{s}$ with respect to a basis of L are coprime). The covector $\boldsymbol{\sigma}$ specifies the invariant plane of the shear since $S(\mathbf{x}) = \mathbf{x}$ is equivalent to $\langle\boldsymbol{\sigma}, \mathbf{x}\rangle = 0$. We shall also assume that $\langle\boldsymbol{\sigma}, \mathbf{s}\rangle = 0$, a condition equivalent to $\det(S) = 1$, so that the transformed lattice $S(L)$ has the same density of nodes as L. Furthermore, $S(L)$ contains $\mathbf{s}$ as an irreducible vector so that both lattices share the same bundle of lattice lines parallel to $\mathbf{s}$. The inverse transformation is simply given by $S^{-1} = I - |\mathbf{s}\rangle\langle\boldsymbol{\sigma}|$.

The mapping S is unbounded in the sense that $S(\mathbf{x}) - \mathbf{x}$ diverges when $\mathbf{x}$ runs over L. For this reason, such a mapping can hardly be accepted as a model of a structural transformation between two lattices. Therefore, 'fractional' shears were introduced (Duneau & Oguey, 1991; Duneau, 1992) as elementary bounded transformations between lattices. The fractional shear $\hat{S}$ associated with S is the (non-linear) mapping defined by

$$\hat{S}(\mathbf{x}) = \mathbf{x} + \mathrm{frac}[\langle\boldsymbol{\sigma}, \mathbf{x}\rangle]\mathbf{s}, \tag{3}$$

where $\mathrm{frac}[t]$ denotes the fractional part of t, between $-1/2$ and $1/2$, so that $t = \mathrm{rnd}[t] + \mathrm{frac}[t]$, where $\mathrm{rnd}[t]$ denotes the nearest integer.

The relationship between S and $\hat{S}$ is given by $\hat{S}(\mathbf{x}) = S(\mathbf{x}) - \mathrm{rnd}[\langle\boldsymbol{\sigma}, \mathbf{x}\rangle]\mathbf{s}$. Since $\mathbf{s}$ belongs to L and $S(L)$, we see that the fractional shear $\hat{S}$ also maps L onto $S(L)$. The displacement field associated with the fractional shear is $\hat{S}(\mathbf{x}) - \mathbf{x} = \mathrm{frac}[\langle\boldsymbol{\sigma}, \mathbf{x}\rangle]\mathbf{s}$. It is bounded by $\|\mathbf{s}\|/2$ so that $\hat{S}$ is a bounded one-to-one mapping between L and $S(L)$. So, for each factorization of the transition matrix T between two lattices, there exists a corresponding bounded transformation between them.

3. The double shear condition

3.1. *Double shear condition*

In this section, we give a simple geometric characterization for the existence of a double shear transformation between two lattices of equal density of nodes. Let L_a and L_b be two such lattices given in standard orientations, for instance cubic lattices with axes parallel to the standard basis vectors of space. We want to determine those rotations R that bring L_b into a position such that L_a and RL_b are related by a double shear.

The result of the present analysis is that the double shear property is equivalent to the existence of a rotation R such that:

(i) One can find some irreducible reciprocal vectors $\mathbf{q}_a$ of L_a^* and $\mathbf{q}_b$ of L_b^* such that $\mathbf{q}_a = R\mathbf{q}_b$. We will write $\mathbf{q}_a = R\mathbf{q}_b = \mathbf{q}$.

(ii) There exist two irreducible vectors $\mathbf{s}_a \in L_a$ and $\mathbf{s}_b \in L_b$ for which $\mathbf{s}_a \times R\mathbf{s}_b = \pm\Gamma\Omega\mathbf{q}$, where Γ is a positive integer and Ω is the common volume of the unit cells.

In order to simplify the notation, we will write $L'_b = RL_b$, $L'^*_b = RL^*_b$ and, in general, $\mathbf{x}' = R\mathbf{x}$ for $\mathbf{x}$ in L_b or L^*_b.

We will prove the above statement which can be written in short as

double shear property between L_a and RL_b

$\Longleftrightarrow \exists$ a rotation R:

$$(1)\ \exists\ \mathbf{q}_a \in L^*_a, \quad \mathbf{q}_b \in L^*_b: \quad \mathbf{q}_a = R\mathbf{q}_b = \mathbf{q};$$

$$(2)\ \exists\ \mathbf{s}_a \in L_a, \quad \mathbf{s}_b \in L_b: \quad \mathbf{s}_a \times R\mathbf{s}_b = \pm\Gamma\Omega_{\mathbf{q}}. \tag{4}$$

Proof.

(*a*) $\Longrightarrow$: Assume first that L_a and L'_b are related by a double shear. This is equivalent to the existence of an 'intermediate' lattice Λ (see Fig. 1), which is a simple shear deformation of both L_a (by the shear $S_a = I + |\mathbf{s}_a\rangle\langle\boldsymbol{\sigma}_a|$) and L'_b (by the shear $S'_b = I + |\mathbf{s}'_b\rangle\langle\boldsymbol{\sigma}'_b|$):

$$L_a \xrightarrow{S_a} \Lambda \xleftarrow{S'_b} L'_b. \tag{5}$$

The shear vector $\mathbf{s}_a$ is an irreducible vector of L_a and Λ; similarly, $\mathbf{s}'_b$ is an irreducible vector of L'_b and Λ. The covectors $\boldsymbol{\sigma}_a$ and $\boldsymbol{\sigma}'_b$ satisfy the orthogonality condition $\langle\boldsymbol{\sigma}_a, \mathbf{s}_a\rangle = \langle\boldsymbol{\sigma}'_b, \mathbf{s}'_b\rangle = 0$.

Since $\mathbf{s}_a$ and $\mathbf{s}'_b$ belong to Λ, they span a lattice plane† P of Λ. Now, as S_a maps L_a onto Λ, the plane $(S_a)^{-1}(P)$

† If $\mathbf{s}_a$ and $\mathbf{s}'_b$ were collinear, L_a and L'_b would be related by a unique shear.

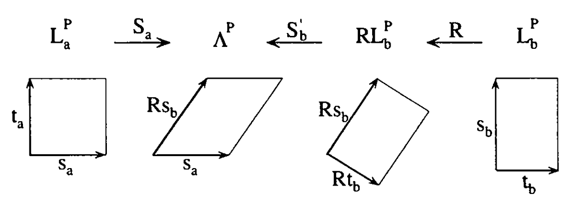

Fig. 1. For certain rotations R, L_a and $L'_b = RL_b$ are related by a double shear, *i.e.* there exists an intermediate lattice Λ such that $\Lambda = S_aL_a = S'_bL'_b$. The figure illustrates the situation in a plane P perpendicular to the rotation axis $\mathbf{q}$.

is a lattice plane of L_a. This plane is spanned by the two vectors $(S_a)^{-1}(\mathbf{s}_a) = \mathbf{s}_a$ and $(S_a)^{-1}(\mathbf{s}'_b) = \mathbf{s}'_b - \langle \boldsymbol{\sigma}_a, \mathbf{s}'_b\rangle \mathbf{s}_a$ of L_a. Therefore, $(S_a)^{-1}(P) = P$ so that P is also a lattice plane of L_a. Likewise, one easily checks that P is a lattice plane of L'_b. Besides, any lattice plane of Λ parallel to P is also invariant by S_a and S'_b. Consequently, the three lattices L_a, L'_b and Λ lie on a common stack of parallel lattice planes. The dual lattices L_a^*, $L_b'^*$ and Λ^* therefore have a common irreducible reciprocal vector $\mathbf{q}$ normal to P and this gives the first necessary condition:

$$\exists\ \mathbf{q}_a \in L_a^*,\quad \mathbf{q}_b \in L_b^*:\quad \mathbf{q}_a = \mathbf{q}'_b = \mathbf{q}, \tag{6}$$

where $\mathbf{q}'_b = R\mathbf{q}_b$.

Furthermore, there exists a basis $\{\mathbf{u}_a, \mathbf{v}_a, \mathbf{w}_a\}$ of L_a and a basis $\{\mathbf{u}'_b, \mathbf{v}'_b, \mathbf{w}'_b\}$ of L'_b such that $\{\mathbf{v}_a, \mathbf{w}_a\}$ forms a basis of the 2D lattice $L_a^P = L_a \cap P$ (L_a^P is the intersection of L_a with the plane P) and $\{\mathbf{v}'_b, \mathbf{w}'_b\}$ is a basis of $L_b'^P = L'_b \cap P$. Let $\Omega = (\mathbf{u}_a, \mathbf{v}_a, \mathbf{w}_a) = (\mathbf{u}'_b, \mathbf{v}'_b, \mathbf{w}'_b)$ denote the common volume of the unit cells of L_a and L'_b. The reciprocal vectors $\mathbf{q}_a$ and $\mathbf{q}'_b$ are then given by $\mathbf{q}_a = \Omega^{-1}(\mathbf{v}_a \times \mathbf{w}_a)$ and $\mathbf{q}'_b = \Omega^{-1}(\mathbf{v}'_b \times \mathbf{w}'_b)$ and satisfy $\langle \mathbf{q}_a, \mathbf{u}_a\rangle = \langle \mathbf{q}'_b, \mathbf{u}'_b\rangle = 1$.

The unit cells of the 2D lattices L_a^P, $L_b'^P$ and Λ^P have the same area $A = |\mathbf{v}_a \times \mathbf{w}_a| = |\mathbf{v}'_b \times \mathbf{w}'_b| = |S_a(\mathbf{v}_a) \times S_a(\mathbf{w}_a)| = \Omega|\mathbf{q}_a| = \Omega|\mathbf{q}'_b| = \Omega|\mathbf{q}|$ and consequently their 2D lattices have the same density of nodes. Since the two vectors $\mathbf{s}_a$ and $\mathbf{s}'_b$ belong to Λ^P, they span a sublattice of Λ^P. This gives rise to the second condition:

$$\exists\ \mathbf{s}_a \in L_a,\quad \mathbf{s}_b \in L_b:\quad \mathbf{s}_a \times \mathbf{s}'_b = \pm\Gamma\Omega\mathbf{q} \tag{7}$$

with $\mathbf{s}'_b = R\mathbf{s}_b$ and where the positive integer Γ denotes the index of this sublattice with respect to Λ^P.

(b) $\Longleftarrow$: Now let us assume that the above conditions (6) and (7) are fulfilled, *i.e.* there exists a rotation R such that $\mathbf{q}_a = \mathbf{q}'_b = \mathbf{q}$ and $\mathbf{s}_a \times \mathbf{s}'_b = \pm\Gamma\Omega\mathbf{q}$. We will show that L_a can be mapped onto L'_b by a double shear $(S'_b)^{-1}S_a$, where again $S_a = I + |\mathbf{s}_a\rangle\langle\boldsymbol{\sigma}_a|$ and $S'_b = I + |\mathbf{s}'_b\rangle\langle\boldsymbol{\sigma}'_b|$. As mentioned above, this is equivalent to the existence of an intermediate lattice Λ between L_a and L'_b, which is $\Lambda = S_aL_a = S'_bL'_b$.

By (6), the vector $\mathbf{q}$ is normal to a plane P of L_a and L'_b. We can choose a vector $\mathbf{t}_a$ in L_a such that $\mathbf{s}_a$ and $\mathbf{t}_a$ form a basis of L_a^P yielding $\mathbf{s}_a \times \mathbf{t}_a = \Omega\mathbf{q}$ and similarly a vector $\mathbf{t}'_b$ in $L_b'^P$ giving $\mathbf{t}'_b \times \mathbf{s}'_b = \Omega\mathbf{q}$.

The existence of a double shear corresponds to the fact that the sheared basis $\{\mathbf{s}_a, S_a(\mathbf{t}_a)\}$ and $\{\mathbf{s}'_b, S'_b(\mathbf{t}'_b)\}$ span the same 2D lattice Λ^P. $S_a(\mathbf{t}_a)$ lies on a line parallel to $\mathbf{s}_a$ at $\mathbf{t}_a$ and, similarly, $S'_b(\mathbf{t}'_b)$ lies on a line parallel to $\mathbf{s}'_b$ at $\mathbf{t}'_b$ (see the dashed lines parallel to $\mathbf{s}_a$ and $\mathbf{s}'_b$ in Fig. 2, which illustrates the case $\Gamma = 2$). The intersection of these lines defines the vector $\boldsymbol{\tau} = \Gamma^{-1}(\mathbf{s}_a + \mathbf{s}'_b)$ forming a basis with $\mathbf{s}_a$ as well as with $\mathbf{s}'_b$, *i.e.* $\mathbf{s}_a \times \boldsymbol{\tau} = \Omega\mathbf{q}$ and $\boldsymbol{\tau} \times \mathbf{s}'_b = \Omega\mathbf{q}$. Thus, we can assume that $S_a(\mathbf{t}_a) = S'_b(\mathbf{t}'_b) = \boldsymbol{\tau}$.

Finally, it remains to completely specify the shears S_a and S'_b in terms of $\boldsymbol{\sigma}_a$ and $\boldsymbol{\sigma}'_b$. The following equations fully characterize $\boldsymbol{\sigma}_a$ and $\boldsymbol{\sigma}'_b$ by means of scalar products:

$$\begin{array}{lllll}
(1a) & \langle \boldsymbol{\sigma}_a, \mathbf{s}_a\rangle = 0 & & \\
(1b) & \langle \boldsymbol{\sigma}'_b, \mathbf{s}'_b\rangle = 0 & & \\
(2a) & S_a(\mathbf{t}_a) = \boldsymbol{\tau} & \Longleftrightarrow & \mathbf{t}_a + \langle \boldsymbol{\sigma}_a, \mathbf{t}_a\rangle \mathbf{s}_a = \boldsymbol{\tau} \\
(2b) & S'_b(\mathbf{t}'_b) = \boldsymbol{\tau} & \Longleftrightarrow & \mathbf{t}'_b + \langle \boldsymbol{\sigma}'_b, \mathbf{t}'_b\rangle \mathbf{s}'_b = \boldsymbol{\tau} \\
(3) & S_a(\mathbf{u}_a) = S'_b(\mathbf{u}'_b) & \Longleftrightarrow & \mathbf{u}_a + \langle \boldsymbol{\sigma}_a, \mathbf{u}_a\rangle \mathbf{s}_a \\
 & & & \quad = \mathbf{u}'_b + \langle \boldsymbol{\sigma}'_b, \mathbf{u}'_b\rangle \mathbf{s}'_b
\end{array} \tag{8}$$

with $\boldsymbol{\tau} = \Gamma^{-1}(\mathbf{s}_a + \mathbf{s}'_b)$. The intermediate lattice Λ is spanned by $\mathbf{s}_a$, $\boldsymbol{\tau}$ and $S_a(\mathbf{u}_a)$ [or by $\mathbf{s}'_b$, $\boldsymbol{\tau}$ and $S'_b(\mathbf{u}'_b)$].

Additionally, we will optimize S_a and S'_b so that the shear amplitudes are as small as possible. The choice of the vector $\mathbf{t}_a$ which forms a basis with $\mathbf{s}_a$ is not completely determined because any vector of the form $\mathbf{t}_a + n\,\mathbf{s}_a$, where n is an integer, is convenient, too. The same is true for any vector $\mathbf{t}'_b + n'\,\mathbf{s}'_b$ forming a basis of $L_b'^P$ with $\mathbf{s}'_b$, where n' is again an integer. In order to have small shear amplitudes, we will choose n and n' such that $|\langle \boldsymbol{\sigma}_a, \mathbf{t}_a + n\,\mathbf{s}_a\rangle| \le \frac{1}{2}$ and $|\langle \boldsymbol{\sigma}'_b, \mathbf{t}'_b + n'\,\mathbf{s}'_b\rangle| \le \frac{1}{2}$. We find:

$$\begin{aligned}
n &= \mathrm{rnd}\{[(\boldsymbol{\tau}, \mathbf{s}_a) - (\mathbf{t}_a, \mathbf{s}_a)]/s_a^2\} \\
n' &= \mathrm{rnd}\{[(\boldsymbol{\tau}, \mathbf{s}'_b) - (\mathbf{t}'_b, \mathbf{s}'_b)]/s_b'^2\}.
\end{aligned} \tag{9}$$

It follows that

$$\begin{aligned}
\langle \boldsymbol{\sigma}_a, \mathbf{t}_a + n\,\mathbf{s}_a\rangle &= \mathrm{frac}\{[(\boldsymbol{\tau}, \mathbf{s}_a) - (\mathbf{t}_a, \mathbf{s}_a)]/s_a^2\} \equiv \xi_a \\
\langle \boldsymbol{\sigma}'_b, \mathbf{t}'_b + n'\,\mathbf{s}'_b\rangle &= \mathrm{frac}\{[(\boldsymbol{\tau}, \mathbf{s}'_b) - (\mathbf{t}'_b, \mathbf{s}'_b)]/s_b'^2\} \equiv \xi'_b.
\end{aligned} \tag{10}$$

Solving the third relation of (8), we get:

$$\begin{aligned}
\langle \boldsymbol{\sigma}_a, \mathbf{u}_a\rangle &= [(\mathbf{u}'_b - \mathbf{u}_a, \mathbf{s}_a)s_b'^2 - (\mathbf{u}'_b - \mathbf{u}_a, \mathbf{s}'_b)(\mathbf{s}_a, \mathbf{s}'_b)] \\
&\quad \times [s_a^2 s_b'^2 - (\mathbf{s}_a, \mathbf{s}'_b)^2]^{-1} \\
&\equiv \zeta_a \\
\langle \boldsymbol{\sigma}_b, \mathbf{u}'_b\rangle &= -[(\mathbf{u}'_b - \mathbf{u}_a, \mathbf{s}'_b)s_a^2 - (\mathbf{u}'_b - \mathbf{u}_a, \mathbf{s}_a)(\mathbf{s}_a, \mathbf{s}'_b)] \\
&\quad \times [s_a^2 s_b'^2 - (\mathbf{s}_a, \mathbf{s}'_b)^2]^{-1} \\
&\equiv \zeta'_b.
\end{aligned} \tag{11}$$

In summary, the following equations determine $\boldsymbol{\sigma}_a$ and $\boldsymbol{\sigma}'_b$:

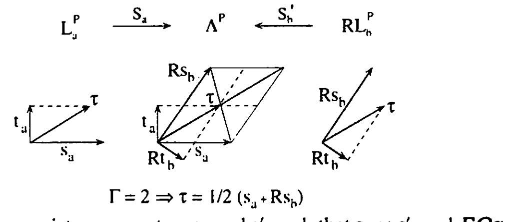

Fig. 2. If there exist some vectors $\mathbf{s}_a$ and $\mathbf{s}'_b$ such that $\mathbf{s}_a \times \mathbf{s}'_b = \pm\Gamma\Omega\mathbf{q}$, the existence of an intermediate lattice Λ is ensured and the double shear property between L_a and L'_b follows. In the plane P, Λ^P is either spanned by $\mathbf{s}_a$ and $\boldsymbol{\tau}$ or by $\mathbf{s}'_b$ and $\boldsymbol{\tau}$ with $\boldsymbol{\tau} = \Gamma^{-1}(\mathbf{s}_a + \mathbf{s}'_b)$. The lattice spanned by $\mathbf{s}_a$ and $\mathbf{s}'_b$ is a sublattice with index Γ with respect to Λ^P. The figure corresponds to $\Gamma = 2$.

$$\begin{array}{llll} (1a) & \langle \boldsymbol{\sigma}_a, \mathbf{s}_a \rangle = 0 & (1b) & \langle \boldsymbol{\sigma}'_b, \mathbf{s}'_b \rangle = 0 \\ (2a) & \langle \boldsymbol{\sigma}_a, \mathbf{t}_a \rangle = \xi_a & (2b) & \langle \boldsymbol{\sigma}'_b, \mathbf{t}'_b \rangle = \xi'_b \\ (3a) & \langle \boldsymbol{\sigma}_a, \mathbf{u}_a \rangle = \zeta_a & (3b) & \langle \boldsymbol{\sigma}'_b, \mathbf{u}'_b \rangle = \zeta'_b. \end{array} \qquad (12)$$

This analysis clearly shows that the double shear conditions (6) and (7) specify particular orientational relationships associated with a rotation R. If the shear vectors $\mathbf{s}_a$ and $\mathbf{s}_b$ are reasonably small and the index Γ bounded, only finitely many solutions can be found. It must be noticed that, even for cubic lattices, such simple solutions may lead to irrational relative orientations with no coincidence lattice.

3.2. *Example of the* $\langle hkl \rangle$ *rotations in a cubic system*

In this section, we analyse the rational orientational relationships in a cubic lattice resulting from the double shear condition. As proved by Duneau, Oguey & Thalal (1992), all relationships associated with a coincidence site lattice fall into the double shear case (note, however, that the inverse is not true in general). The existence of a CSL requires that the transition matrix T mapping a basis of the lattice L_a onto a basis of the lattice L'_b is rational (Warrington & Bufalini, 1971; Grimmer, 1976). Thus, if we assume L_a and L_b equal to $\mathbf{Z}^3$ ($\Omega = 1$), the transition matrix T is equal to the rotation matrix R. Therefore, if R is rational, we need at most two nontrivial shears to map L_a onto L'_b.

Now the rotation axis is specified by a reciprocal vector $\mathbf{q} = \langle hkl \rangle$ normal to the plane P that contains the shear vectors $\mathbf{s}_a$ and $\mathbf{s}'_b$. The rotation angle φ of R is such that the cell spanned by $\mathbf{s}_a$ and $\mathbf{s}'_b$ has an area $A = \Gamma|\mathbf{q}|$, where $|\mathbf{q}| = (h^2 + k^2 + l^2)^{1/2}$ and $\Omega = 1$. If θ is the angle between $\mathbf{s}_a$ and $\mathbf{s}'_b$ (see Fig. 3), the condition (7) reads

$$|\mathbf{s}_a||\mathbf{s}'_b| \sin(\theta) = \lambda \Gamma |\mathbf{q}| = \lambda \Gamma (h^2 + k^2 + l^2)^{1/2}, \qquad (13)$$

where $\lambda = \pm 1$.

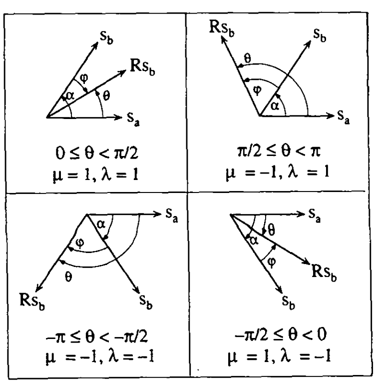

Fig. 3. The angle between $\mathbf{s}_a$ and $\mathbf{s}_b$ is denoted by α, the one between $\mathbf{s}_a$ and $\mathbf{s}'_b$ by θ so that we have $\varphi = \theta - \alpha$ for the rotation angle φ. The variables λ and μ are given by $\sin(\theta) = \lambda|\sin(\theta)|$ and $\cos(\theta) = \mu|\cos(\theta)|$. Depending on the angle θ, λ and μ can take the values $+1$ and -1 and consequently one gets four different values of φ for given $\mathbf{q}$, $|\mathbf{s}_a|$, $|\mathbf{s}_b|$, α and Γ.

If α denotes the angle between $\mathbf{s}_a$ and $\mathbf{s}_b$, then $\varphi = \theta - \alpha$. The above formula therefore gives all possible rotation angles φ depending on $\mathbf{q}$, α, $|\mathbf{s}_a|$, $|\mathbf{s}_b|$ and Γ. In the following, we will select those Γ, $\mathbf{s}_a$ and $\mathbf{s}_b$ for which the rotation matrix R is rational and therefore yields a 3D coincidence lattice $L_a \cap L'_b$. Then, we will show how to compute the corresponding Σ.

First, we calculate the 3D rotation matrix R in a basis $\{\mathbf{u}, \mathbf{v}, \mathbf{w}\}$ common to both cubic lattices L_a and L_b and adapted to our problem. The vectors $\mathbf{v}$ and $\mathbf{w}$ span the plane P normal to the rotation axis $\mathbf{q}$.

The action of a rotation R about an axis $\mathbf{q}$ through an angle φ is given by

$$\begin{aligned} R\mathbf{x} = {} & [(\mathbf{q}, \mathbf{x})/q^2]\mathbf{q} + \cos(\varphi)\{\mathbf{x} - [(\mathbf{q}, \mathbf{x})/q^2]\mathbf{q}\} \\ & + [\sin(\varphi)/|\mathbf{q}|]\mathbf{q} \times \mathbf{x}. \end{aligned} \qquad (14)$$

The matrix entries of R in the basis $\{\mathbf{u}, \mathbf{v}, \mathbf{w}\}$ can be deduced from

$$\begin{aligned} R\mathbf{u} &= \mathbf{u} + \{F[1 - \cos(\varphi)]/q^2 - B\sin(\varphi)/|\mathbf{q}|\}\mathbf{v} \\ &\quad + \{G[1 - \cos(\varphi)]/q^2 + A\sin(\varphi)/|\mathbf{q}|\}\mathbf{w} \\ R\mathbf{v} &= [\cos(\varphi) - D\sin(\varphi)/|\mathbf{q}|]\mathbf{v} + C[\sin(\varphi)/|\mathbf{q}|]\mathbf{w} \\ R\mathbf{w} &= -E[\sin(\varphi)/|\mathbf{q}|]\mathbf{v} + [\cos(\varphi) + D\sin(\varphi)/|\mathbf{q}|]\mathbf{w}, \end{aligned} \qquad (15)$$

where A, B, C, D, E, F and G are integers given by $A = (\mathbf{u}, \mathbf{v})$, $B = (\mathbf{u}, \mathbf{w})$, $C = (\mathbf{v}, \mathbf{v})$, $D = (\mathbf{v}, \mathbf{w})$, $E = (\mathbf{w}, \mathbf{w})$, $F = BD - AE$ and $G = AD - BC$.

Now one can see that the rationality of the rotation matrix R is equivalent to the rationality of $\cos(\varphi)$ and $\sin(\varphi)/|\mathbf{q}|$. From (13), we have $\sin(\theta) = \lambda\Gamma|\mathbf{q}|/|\mathbf{s}_a||\mathbf{s}_b|$ and $\cos(\theta) = \mu[1 - \sin^2(\theta)]^{1/2}$, where $\lambda = \pm 1$ and $\mu = \pm 1$. For given $\mathbf{s}_a$ and $\mathbf{s}_b$, we can calculate $\cos(\alpha) = (\mathbf{s}_a, \mathbf{s}_b)/|\mathbf{s}_a||\mathbf{s}_b|$ and consequently $\sin(\alpha) = \nu[1 - \cos^2(\alpha)]^{1/2}$, where $\nu = +1$ or -1, depending on whether $\mathbf{s}_a \times \mathbf{s}_b$ is parallel to $\mathbf{q}$ ($\nu = 1$) or antiparallel to $\mathbf{q}$ ($\nu = -1$). Using elementary trigonometry, we can express $\cos(\varphi)$ and $\sin(\varphi)/|\mathbf{q}|$ in terms of $\mathbf{q}$, α, $|\mathbf{s}_a|$, $|\mathbf{s}_b|$ and Γ:

$$\begin{aligned} \cos(\varphi) &= \big(\mu(s_a^2 s_b^2 - \Gamma^2 q^2)^{1/2}(\mathbf{s}_a, \mathbf{s}_b) \\ &\quad + \lambda\nu\Gamma\{q^2[s_a^2 s_b^2 - (\mathbf{s}_a, \mathbf{s}_b)^2]\}^{1/2}\big)/s_a^2 s_b^2 \\ \sin(\varphi)/|\mathbf{q}| &= \big(\lambda\Gamma q^2(\mathbf{s}_a, \mathbf{s}_b) - \mu\nu(s_a^2 s_b^2 - \Gamma^2 q^2)^{1/2} \\ &\quad \times \{q^2[s_a^2 s_b^2 - (\mathbf{s}_a, \mathbf{s}_b)^2]\}^{1/2}\big)/q^2 s_a^2 s_b^2. \end{aligned} \qquad (16)$$

As the value of ν is fixed by $\mathbf{s}_a$ and $\mathbf{s}_b$, one gets four different values of φ for given $\mathbf{q}$, $|\mathbf{s}_a|$, $|\mathbf{s}_b|$, α and Γ, depending on whether λ and μ are $+1$ or -1 (see Fig. 3).

Finally, straightforward calculations show that $\cos(\varphi)$ and $\sin(\varphi)/|\mathbf{q}|$ are rational numbers if and only if the terms $(s_a^2 s_b^2 - \Gamma^2 q^2)^{1/2}$ and $\{q^2[s_a^2 s_b^2 - (\mathbf{s}_a, \mathbf{s}_b)^2]\}^{1/2}$ are both integers. If these conditions on Γ, $\mathbf{s}_a$ and $\mathbf{s}_b$ are met, then the rotation matrix R is irrational. The double shear yields a CSL and the corresponding index Σ can be easily obtained by computation of the l.c.m. of the denominators of $\{R_{ij}\}_{i,j\in\{\mathbf{u},\mathbf{v},\mathbf{w}\}}$.

Table 1 shows an example of rotations about an axis $\mathbf{q} = \langle 0,0,1\rangle$. The basis $\{\mathbf{u},\mathbf{v},\mathbf{w}\}$ is given by $\mathbf{u} = (0,0,1)$, $\mathbf{v} = (1,0,0)$ and $\mathbf{w} = (0,1,0)$. The vectors $\mathbf{v}$ and $\mathbf{w}$ span the plane orthogonal to $\mathbf{q}$ and $\langle \mathbf{q},\mathbf{u}\rangle = 1$. The table gives a systematic list of shear directions $\mathbf{s}_a = m_a\mathbf{v} + n_a\mathbf{w}$ and $\mathbf{s}_b = m_b\mathbf{v} + n_b\mathbf{w}$ for increasing values of Γ, for which the calculated $\cos(\varphi)$ and $\sin(\varphi)/|\mathbf{q}|$ values are rational. In each step, the corresponding rotation angle φ and Σ are calculated. Missing Σ are due to necessary bounds on the indices Γ, $m_{a,b}$ and $n_{a,b}$ given in the computer algorithm (here: $1 \le \Gamma \le 5$ and $0 \le m_{a,b}, n_{a,b} \le 5$). For instance, $\Sigma = 37$ is missing in our table due to the limits on the shear parameters. It can be found for $\Gamma = 1$, $m_a = 1$, $n_a = 0$, $m_b = 6$, $n_b = -1$ and $\varphi = 18.9246$. Table 1 is also limited to rotation angles in the interval $[0, \pi/4]$; this is justified in our example, where the lattices are cubic and the rotation axis $\mathbf{q} = \langle 001\rangle$.

Table 1. *Double shear relationship associated with a CSL with rotation axis* $\mathbf{q} = \langle 001\rangle$

The shear vectors are given by $\mathbf{s}_a = m_a\mathbf{v} + n_a\mathbf{w} = (m_a, n_a, 0)$ and $\mathbf{s}_b = m_b\mathbf{v} + n_b\mathbf{w} = (m_b, n_b, 0)$.

Γ	Σ	m_a	n_a	m_b	n_b	φ
1	5	1	0	2	1	36.8699
1	13	1	1	3	2	22.6199
1	17	1	0	1	4	28.0725
1	25	2	1	3	1	16.2602
1	29	2	1	2	5	43.6028
1	41	1	1	5	4	12.6804
1	65	3	2	2	1	14.2500
1	85	3	1	4	1	8.7974
1	145	5	2	3	1	6.7329
1	145	2	1	5	2	9.5273
1	221	3	2	5	3	5.4526
1	325	4	3	3	2	6.3597
1	1025	5	4	4	3	3.5798
2	85	2	1	4	1	25.0576
2	125	4	3	2	1	20.6097
2	533	5	4	3	2	9.9395
3	65	3	2	3	1	30.5102
3	205	5	4	2	1	24.1895
3	425	4	3	5	3	11.8123
3	493	5	2	4	1	15.5303
4	377	3	2	5	2	23.7773
5	169	3	2	2	3	44.7603
5	221	3	2	4	1	39.3076
5	377	5	2	5	1	20.9830
5	493	5	3	5	2	18.3247
5	697	5	4	5	3	15.3921

4. Single shear transformations and coincidence site lattices for cubic systems

Previously, we have selected those Γ, $\mathbf{s}_a$ and $\mathbf{s}_b$ for which the rotation matrix R is rational and have calculated the corresponding Σ. Now, one can examine the inverse problem, *i.e.* determine the shear transformations for *a priori* given rotation axis $\mathbf{q}$, rotation angle φ and index Σ. It turns out that for the particular case of cubic lattices one single shear transforms L_a into L'_b. We will show how to determine it in principle.

We therefore apply the method developed by Duneau, Oguey & Thalal (1992), especially the theory of Smith normal forms (see Newmann, 1972; Hua Loo Keng, 1982) and a theorem about triangular matrices. As Σ corresponds to the l.c.m. of the denominators of the rotation matrix R, one can see that ΣR is an integer matrix, with entries depending on the rotation angle φ and the adapted basis $\{\mathbf{u},\mathbf{v},\mathbf{w}\}$ [see (15)]. The theorem of Smith ensures that there exist modular matrices U and V (integer matrices with determinant ± 1) such that $\Delta = U(\Sigma R)V$ is a diagonal integer matrix. Such a diagonal Smith matrix is unique and has the following form in the present case:

$$\Delta = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \Sigma & 0 \\ 0 & 0 & \Sigma^2 \end{pmatrix}. \tag{17}$$

The modular matrices U and V are obtained by an algorithm, but are not uniquely defined. Yet another theorem guarantees that one can associate a second pair of modular matrices U' and V' to a diagonal integral matrix Δ such that $\mathcal{J} = U'\Delta V'$ is a triangular matrix with Δ given by (17). U' and V' can be constructed from Δ and we have:

$$U' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \Sigma & 0 & 1 \end{pmatrix} \quad \text{and} \quad V' = \begin{pmatrix} \Sigma & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

$$\Rightarrow \mathcal{J} = \begin{pmatrix} \Sigma & 0 & 1 \\ 0 & \Sigma & 0 \\ 0 & 0 & \Sigma \end{pmatrix}. \tag{18}$$

It follows that

$$\mathcal{J} = \Sigma \begin{pmatrix} 1 & 0 & 1/\Sigma \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \Sigma S, \tag{19}$$

i.e. the triangular matrix $\mathcal{J}$ can be decomposed as the product of Σ and a shear transformation S given by $S = \mathbf{1} + (1/\Sigma)|\mathbf{e}_1\rangle\langle\mathbf{e}_3|$. We eventually get the following relation: $S = \tilde{U} R \tilde{V}$, where $\tilde{U} = U'U$ and $\tilde{V} = V V'$. Expanding $R = \tilde{U}^{-1} S \tilde{U}\, \tilde{U}^{-1}\tilde{V}^{-1}$, one can see that, as $\tilde{U}^{-1}\tilde{V}^{-1}\mathbf{Z}^3 = \mathbf{Z}^3$, the action of R on the lattice $\mathbf{Z}^3$ corresponds to a conjugation of a single shear transformation, which again yields a shear transformation:

$$\tilde{S} = \tilde{U}^{-1} S\, \tilde{U} = \mathbf{1} + (1/\Sigma)|\tilde{U}^{-1}\mathbf{e}_1\rangle\langle\tilde{U}^t\mathbf{e}_3|. \tag{20}$$

5. Comparison with experimental data

In this section, we will briefly explain the experiments performed on bicrystals by Putaux & Thibault-Dessaux

(1990) and compare their results on the rotation angles φ and index Σ of the CSL with our calculations *via* the shear transformations. Putaux & Thibault-Dessaux (1990) first fabricated bicrystals of silicon with symmetric tilt coincidence boundary $\Sigma = 9(122)$ corresponding to a rotation through 38.94° about the rotation axis [0,1,1]. In a second step, these bicrystals were compressed at different temperatures and the resulting Σ of the CSL, the orientational relationship, *i.e.* the angle φ between the two lattices, and their interface were determined.

We have tried to reproduce some of their numerical results by a computer program selecting shear transformations giving the observed Σ and φ analogous to what is shown in Table 1. Table 2 shows the case where we found a unique shear transformation lying in the interface of the two crystals. The table shows the single shear directions $\mathbf{s} = m\mathbf{v} + n\mathbf{w}$ given in the adapted basis $\mathbf{u} = (0, 1, 0)$, $\mathbf{v} = (0, -1, 1)$ and $\mathbf{w} = (1, 0, 0)$ and in standard coordinates. In Table 3, we list the cases where we found two shear transformations with shear directions $\mathbf{s}_a = m_a\mathbf{v} + n_a\mathbf{w}$ and $\mathbf{s}_b = m_b\mathbf{v} + n_b\mathbf{w}$, which have relatively small shear parameters compared with the single shear case and reasonably small Γ values. In both cases, our rotation angle φ and Σ perfectly agree with the experimental data.

6. Conclusions

The transition matrix between two lattices completely describes their orientational relationship. The existence of a coincidence lattice is equivalent to the rationality of this matrix. On the other hand, a matrix of determinant ± 1 can be factorized into a product of at most four shear matrices. We have shown that the rational orientational relationships correspond to a factorization into at most two shear matrices. These cases can be labelled by an integer Γ, which can be related to the coincidence index Σ. The examination of different observations on experimentally produced bicrystals of silicon shows that the very high Σ (up to 337) are actually associated with low Γ ($1 \leq \Gamma \leq 4$). We therefore expect this approach of orientational relationships to have a physical basis. An apparent difficulty with this analysis is that to a given orientational relationship usually more than one interpretation in terms of shear transformations can be given. We believe, however, that these different solutions can be evaluated by considering the geometry of the shear transformations and, in particular, the shear vectors that could be involved in structural transformations. Such an analysis will be given in a future paper.

Table 2. *The unique shear transformations for different CSLs transforming L_a into RL_b*

The shear direction **s** lies at the interface of the two crystals. It is given in the adapted basis $\mathbf{v} = (0, -1, 1)$ and $\mathbf{w} = (1, 0, 0)$ by $\mathbf{s} = m\mathbf{v} + n\mathbf{w}$ and in standard coordinates by $\mathbf{s} = (n, -m, m)$.

Σ	φ	m	n	**s**	Γ
59	45.9795	3	−10	(−10, −3, 3)	1
153	47.6853	5	−16	(−16, −5, 5)	1
187	42.8935	5	−18	(−18, −5, 5)	1
337	44.8302	7	−24	(−24, −7, 7)	1

Table 3. *Double shear transformation with shear directions* $\mathbf{s}_a$ *and* $\mathbf{s}_b$

Choice of relatively small shear parameters (compared with the single shear case) and reasonably small Γ values.

Σ	φ	m_a	n_a	$\mathbf{s}_a$	m_b	n_b	$\mathbf{s}_b$	Γ
59	45.9795	5	3	(3, −5, 5)	2	−1	(−1, −2, 2)	1
153	47.6853	2	−3	(−3, −2, 2)	1	5	(5, −1, 1)	3
187	42.8935	4	1	(1, −4, 4)	2	−3	(−3, −2, 2)	4
337	44.8302	−12	−7	(−7, 12, −12)	5	−3	(−3, −5, 5)	1

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