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Coincidence Lattices and Associated Shear Transformations

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Abstract

A general description of the mutual orientation of two lattices is presented for the cases where the orientation is 'rational'. The coincidence site and displacement-shift complete lattices are genuine lattices whose parameters can be explicitly evaluated through a method based on the Smith normal form for integer matrices. In particular, a formula for the index Σ in terms of the transition matrix is proved to hold true for any symmetry, thereby improving previous statements. Following ideas originally pertaining to the theory of displacive transformations, the transition matrix is analysed in terms of elementary shears. This may serve as a relevant physical criterion for classifying orientations. Applications include the theory of crystal interfaces and grain boundaries as well as structural transitions.

I. Introduction

Beyond the classification of lattices into Bravais classes and crystal systems, which is a classical subject, at least in three dimensions, an important question concerns the classification of pairs of lattices. Such questions are fundamental in the physics of interfaces and grain boundaries, as well as in some problems of structural transitions between crystalline states. Partial answers are provided by the crystallography of coincidence site lattices (CSL) and related displacement-shift complete (DSC) lattices, together with the description of structural units in grain boundaries.

The particular instances yielding complete coincidence lattices – the rational orientations – are of great importance and have been extensively studied both experimentally and theoretically. Cubic systems were the first to be examined (Bollman, 1970; Warrington & Bufalini, 1971; Grimmer, 1971; Pumphrey & Bowket, 1972; Grimmer, Bollmann & Warrington, 1974; Grimmer, 1974, 1976; Bleris & Delavignette, 1981), since they have the advantage that the structure matrices are proportional to the identity. Only recently have other systems such as the hexagonal one (Bonnet, Cousineau & Warrington, 1981; Hagège, 1991) been investigated theoretically.

Most problems studied thus far can be handled in a unified and often shorter way, which is presented in this paper. The main mathematical result we use is the Smith normal form of integral matrices. Although noted by Grimmer (1976), this tool does not seem to have received much attention. The Smith normal form of an integral matrix P is a diagonal integral matrix Δ that satisfies two properties: (i) $P = U\Delta V$, where U and V are modular matrices, and (ii) the diagonal elements are ordered in an increasing way, each being a divisor of the next one. Under these conditions the Smith matrix is unique.

The connexion between lattices and linear algebra is made by specifying a vectorial basis in each lattice. A change of basis within a lattice corresponds to a matrix with integer coefficients and determinant 1. Such matrices constitute a group, $GL(n, \mathbf{Z})$, called the modular group, so all possible bases for a lattice can be indexed by the modular matrices. It follows that algebraic entities are characterized only up to multiplication by such modular matrices: for example, two structure matrices define the same lattice if one is the right product of the other by a modular matrix. Similarly, two transition matrices – accounting for the mutual orientation of two lattices – are equivalent if they satisfy a relation of type (i) mentioned above. Therefore it turns out that the Smith form is an invariant of all equivalent rational transition matrices. This means that it represents geometric properties of the lattices, independent of the particular bases. Moreover, the Smith decomposition is systematic – applies to all rational cases – and completely algorithmic: as will be shown, the computations of, say, the CSL or DSC lattices can be easily

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implemented on a computer (the main step being a procedure returning the greatest common divisor of three integers).

The second purpose of this paper is to develop an alternative approach of orientational relationships between lattices that is based on a decomposition into elementary 'shear' transformations. Duneau & Oguey (1991) showed that the transition matrix between any two lattices of equal density can be decomposed into four shear transformations (in three dimensions). This number four is generic but, for particular and isolated relative orientations, only two shears (or even one shear) suffice to perform the transformation. Such situations are believed to have physical relevance as was recently argued in the case of icosahedral twins where no CSL exists (Duneau, 1990; Duneau & Oguey, 1990).

In the present work we specialize to rational orientations and we will prove that if two n-dimensional lattices are related by a rational transition matrix then they are also related by $n-1$ shear transformations. This leaves us with two shears for the most general (rational) case in three dimensions. These transformations have lattice directions, lattice-invariant planes and rational amplitudes. It follows from a previous study (Duneau & Oguey, 1991) that both lattices are also related by a regular 'displacive' transformation performed by a finite and usually small displacement field.

In § II we recall standard algebraic concepts of n-dimensional crystallography and we define the transition matrices associated with pairs of lattices. In § III, we give a short outline of the Smith normal forms of integral matrices and we consider a first example concerning the transition matrix with $\Sigma = 5$. § IV provides explicit formulae for the intersection lattices (CSL) and sum (DSC) lattices. In § V, we show that any n-dimensional transition matrix is equivalent to a product of at most $n-1$ rational shear matrices. Further results in the two- and three-dimensional cases are presented in § VI.

II. Algebraic concepts in the theory of lattices: a brief summary

1. *N-dimensional crystallography*

An n-dimensional Bravais lattice in the n-dimensional space $\mathbf{R}^n$ is specified by $L_a = A\mathbf{Z}^n$, where A is a regular $n \times n$ matrix called a structure matrix. It defines a basis $(\mathbf{a}) = (\mathbf{a}_1, \ldots, \mathbf{a}_n)$ of L_a through the relation $\mathbf{a}_i = A\mathbf{e}_i = \sum_{j=1}^n A_{ji}\mathbf{e}_j$,

$$\mathbf{a}_1 = A\mathbf{e}_1 = \begin{bmatrix} A_{11} \\ \vdots \\ A_{n1} \end{bmatrix}, \ldots, \mathbf{a}_n = A\mathbf{e}_n = \begin{bmatrix} A_{1n} \\ \vdots \\ A_{nn} \end{bmatrix}, \qquad \text{(II.1)}$$

where $(\mathbf{e}) = (\mathbf{e}_1, \ldots, \mathbf{e}_n)$ denotes the standard basis of $\mathbf{Z}^n$: $\mathbf{e}_1 = (1, 0, \ldots, 0)$ *etc.* Any lattice node $\mathbf{x}$ of L_a is of the form $\mathbf{x} = AX = \sum X_i\mathbf{a}_i$, where X has integer entries. Thus the structure matrix maps the abstract lattice $\mathbf{Z}^n$ in the space of indices onto the physical lattice in real space.

A group isomorphism exists between the point group P of L_a, consisting of all rotations of $SO(n)$ $[O(n)]$ leaving L_a unchanged, and a group of $n \times n$ matrices with integral entries and determinant 1 (± 1). Thus if ρ belongs to the point group P then $\rho\mathbf{a}_1, \rho\mathbf{a}_2, \ldots, \rho\mathbf{a}_n$ belong to L_a, actually constituting a new basis; the integral representation g is provided by the components of $\rho\mathbf{a}_i$ in the former basis $(\mathbf{a})$: $\rho\mathbf{a}_i = \sum g_{ji}\mathbf{a}_j$. In other words, ρ and g are conjugates: $g = A^{-1}\rho A$ and $\det(g) = \det(\rho)$. An 'arithmetic group' G is defined by $G = A^{-1}PA = \{g = A^{-1}\rho A \mid \rho$ in $P\}$; G is isomorphic to P by means of the conjugacy. G contains only $n \times n$ integral matrices with determinant ± 1, so it is a subgroup of the modular group $\mathrm{GL}(n, \mathbf{Z})$.

However, the basis $(\mathbf{a})$ is not unique and infinitely many different bases of L_a exist, each being associated with structure matrices A' of the form $A' = AU$ where U is a modular matrix. Obviously, $L_a = AU\mathbf{Z}^n$. The corresponding arithmetic group is $G' = A'^{-1}PA' = U^{-1}GU$, so that G' is conjugated to G in the modular group. In summary, each lattice L_a is associated with a unique conjugacy class $\Gamma = \{U^{-1}GU, U$ in $\mathrm{GL}(n, \mathbf{Z})\}$. For example, there are 73 such classes in the modular group $\mathrm{GL}(3, \mathbf{Z})$.

2. *The mutual orientation of two lattices*

The orientational relationships between two lattices L_a and L_b such that a coincidence lattice exists correspond to rotations ρ such that $g = A^{-1}\rho A$ is a rational matrix (a matrix with rational entries). Such a property was first pointed out as pertaining to the matrix rotation ρ itself in the case of cubic lattices (Warrington & Bufalini, 1971). For more general lattices, only the conjugated matrix $g = A^{-1}\rho A$ satisfies this property. For simple cases only, the smallest integer μ such that μg is an integral matrix is precisely the index Σ associated with the coincidence site lattice (CSL) (Grimmer, Bollmann & Warrington, 1974, and references therein; Grimmer, 1974).

A transition matrix T from L_a to another lattice L_b is a matrix such that $L_b = AT\mathbf{Z}^n$. Such a matrix always exists and can be obtained as follows: given a basis $(\mathbf{b}) = (\mathbf{b}_1, \ldots, \mathbf{b}_n)$ of L_b, an $n \times n$ array of real numbers (T_{ij}) is deduced from the decomposition of $(\mathbf{b})$ with respect to $(\mathbf{a})$,

$$\mathbf{b}_i = \sum_{j=1}^n T_{ji}\mathbf{a}_j. \qquad \text{(II.2)}$$

If B is the structure matrix defined by $\mathbf{b}_i = B\mathbf{e}_i = \sum_{j=1}^n B_{ji}\mathbf{e}_j$, this equation means that $B = AT$. So the transition matrix is related to the structure matrices by

$$T = A^{-1}B. \qquad \text{(II.3)}$$

As mentioned in the *Introduction*, the structure matrices depend on the choice of the bases (**a**) and (**b**). If U and V are modular matrices then $L_a = AU\mathbf{Z}^n$, $L_b = BV\mathbf{Z}^n$ and the new transition matrix is $T' = U^{-1}TV$: the two matrices T and T' are equivalent.

From (II.3) we have $\det(T) = \det(B)/\det(A)$, meaning that $\det(T)$ is the relative density of L_a with respect to L_b. In particular, L_a and L_b have the same density if and only if $\det(T) = \pm 1$; if, furthermore, T has integer entries, then T is a modular matrix and $L_b = L_a$.

The intersection $L_a \cap L_b$ is defined as the set of nodes belonging to both lattices. The sum $L_a + L_b$ is the set of points $x + y$ where x is in L_a and y is in L_b. $L_a + L_b$ is generated by the $2n$ vectors $(\mathbf{a}_1, \ldots, \mathbf{a}_n, \mathbf{b}_1, \ldots, \mathbf{b}_n)$, which are, of course, linearly dependent.

In general, the intersection of L_a and L_b reduces to the origin $\{0\}$ and the sum is a dense set of points in space. This sum is actually a $\mathbf{Z}$ module, as pointed out and used by Gratias & Thalal (1988). This generic case is met if, for instance, L_a is the two-dimensional square lattice $\mathbf{Z}^2$ spanned by $\mathbf{a}_1 = (1, 0)$ and $\mathbf{a}_2 = (0, 1)$, whereas L_b is rotated from L_a by $\pi/4$. These situations are also characterized by transition matrices having only irrational entries. Intermediate situations, where T has both rational and irrational entries, may also occur. Such irrational cases were studied by Duneau & Oguey (1991) and will not be discussed here.

We will consider only transition matrices T with rational entries. This implies that L_a and L_b have a full coincidence lattice in the sense that $L_a \cap L_b$ is an n-dimensional sublattice of both L_a and L_b, usually referred to as the CSL (coincidence site lattice). In this case the sum lattice $L_a + L_b$ is also an n-dimensional lattice - without any cluster points - usually called the DSC (displacement-shift complete) lattice.

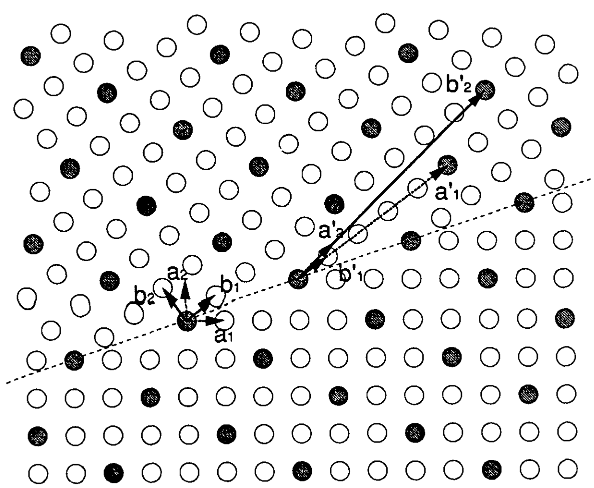

Fig. 1. The $\Sigma = 5$ geometry of a square lattice corresponds to a rotation angle of approximately 36.87°. The standard bases are $\{\mathbf{a}_1, \mathbf{a}_2\}$ and $\{\mathbf{b}_1, \mathbf{b}_2\}$. The proportional bases provided by means of the Smith normal form are $\{\mathbf{a}'_1, \mathbf{a}'_2\}$ and $\{\mathbf{b}'_1, \mathbf{b}'_2\}$ with $\mathbf{a}'_1 = 5\mathbf{b}'_1$ and $5\mathbf{a}'_2 = \mathbf{b}'_2$. The coincidence lattice is shown by the dark circles.

If L_b is identical with L_a up to a rotation R then $B = RA$ and the transition matrix is equal to $A^{-1}RA$. Transition matrices of this form are rational only when associated with particular rotations or orientations. We see that, once a structure matrix A is given, these rational transition matrices belong to a subgroup Γ of the group $\mathrm{SL}(n, \mathbf{Q})$ of rational matrices with determinant ± 1: Γ contains all the matrices of $\mathrm{SL}(n, \mathbf{Q})$ that are conjugate, by A, to some rotation R. Γ is usually infinite; it is isomorphic to a subgroup Π of the rotations $O(n)$ that includes, in particular, the point group P; thus Γ contains the arithmetic group G defined above.

Example. We consider the well known geometry of the $\Sigma = 5$ grain boundary in the (001) plane of a cubic lattice (Bacmann, Papon, Petit & Sylvestre, 1985). The two-dimensional square lattice L_a is given by

$$L_a = A\mathbf{Z}^2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \mathbf{Z}^2. \tag{II.4}$$

The second lattice L_b is rotated with respect to L_a by a rotation R of angle $\cos^{-1} 4/5 \simeq 36.87°$ (see Fig. 1),

$$R = \tfrac{1}{5} \begin{bmatrix} 4 & -3 \\ 3 & 4 \end{bmatrix}. \tag{II.5}$$

Therefore $B = RA$ and

$$L_b = B\mathbf{Z}^2 = \tfrac{1}{5} \begin{bmatrix} 4 & -3 \\ 3 & 4 \end{bmatrix} \mathbf{Z}^2. \tag{II.6}$$

The (rational) transition matrix $T = A^{-1}B$ is given by

$$T = \tfrac{1}{5} \begin{bmatrix} 4 & -3 \\ 3 & 4 \end{bmatrix}. \tag{II.7}$$

In one dimension, finding the intersection and sum lattices reduces to number-theoretic investigations: if $L_a = \alpha\mathbf{Z}$ and $L_b = \beta\mathbf{Z}$ denote two sublattices of $\mathbf{Z}$ with α and β positive integers then the intersection lattice, $L_a \cap L_b = \mathrm{l.c.m.}(\alpha, \beta)\mathbf{Z}$, is spanned by the least common multiple of α and β and the sum lattice, $L_a + L_b = \mathrm{g.c.d.}(\alpha, \beta)\mathbf{Z}$, is spanned by their greatest common divisor.

In higher dimensions, finding explicit bases (equivalently, structure matrices) for the CSL and DSC lattices is not a trivial matter. We will give a procedure based on the Smith normal form. This will be achieved in three steps. Firstly, we restate Smith's theorem and mention some properties of the S-normal form (§ III.1). Next, given an arbitrary rational transition matrix T, we extract from it an integer matrix P (§ III.2). Translated into geometrical language, the Smith form provides 'proportional' bases of the lattices L_a, L_b in terms of which finding the intersection and sum lattices reduces to a sequence of independent one-dimensional problems. Finally, the solutions are presented in § IV for the CSL and the DSC.

III. Smith form of the transition matrix

1. *Smith's theorem*

The theory of the Smith normal form of integral matrices is given by, for example, Newmann (1972) and Hua Loo Keng (1982). We only give a short outline here. The principal result is given by the following theorem.

Theorem. For any $n\times n$ integral matrix A, there exist modular matrices U and V (matrices with integral entries and determinant ± 1) such that UAV is a diagonal matrix Δ. Furthermore, if the rank of A is r, Δ can be found such that the only nonvanishing entries are the positive diagonal elements $\delta_1, \delta_2, \ldots, \delta_r$ that satisfy the property: δ_k divides δ_{k+1} for $k=1$ to $r-1$. Such a diagonal form is then unique.

Outline of the proof. The procedure for transforming A into a diagonal matrix makes use of elementary modular matrices that perform the following operations:

(1) interchange of two rows (columns);

(2) addition of n times one row (column) to another row (column).

(3) multiplication of a row (column) by -1.

A first stage is the following: If $a_1, a_2, \ldots, a_n$ are coprime integers (*i.e.* with g.c.d. $=1$), there exists a modular matrix U with first row (first column) equal to $(a_1, a_2, \ldots, a_n)$. Consequently, if A has a first row (column) with g.c.d. equal to δ, one can find a modular matrix U such that AU (UA) has its first row (column) equal to $(\delta, 0, \ldots, 0)$.

Then the algorithm giving the Smith decomposition proceeds by induction on the dimension n.

Using elementary modular matrices, a nonzero element of A can be brought to position (1, 1). This element can be replaced by the g.c.d. of the first row and then by the g.c.d. of the first column so that it divides all elements of the first row and the first column. Then all other elements of the first row and column can be made zero. If the new element (1, 1) does not divide some other element (i,j) then add column j to column 1 and repeat the first step until the element (1, 1) divides all the other ones. At this point, we are left with an $(n-1)$-dimensional problem that is handled in the same way.

For any $n\times n$ integral matrix A, the determinantal divisors $d_k(A)$ are defined for $k=0, 1, \ldots, n$ by $d_0(A)=1$ and $d_k(A)$ is the greatest common divisor of all the $k\times k$ minors of A. In particular, we have $d_1(A)=\text{g.c.d.}\{A_{ij}\}$ and $d_n(A)=\det(A)$. It can easily be seen that d_{k-1} divides d_k. Now, if U and V are modular matrices and if $B=UAV$, then $d_k(A)=d_k(B)$; this follows from the Binet-Cauchy theorem, which implies that the $k\times k$ minors of B are integral combinations of $k\times k$ minors of A and *vice versa.* Applying this remark to A and its Smith normal form Δ, we find that the diagonal entries $\delta_1, \delta_2, \ldots, \delta_n$ of Δ satisfy the relations $\delta_1=d_1(A)$, $\delta_1\delta_2=d_2(A), \ldots$, $\delta_1\delta_2\ldots\delta_n=d_n(A)$.

Two conclusions can be drawn: (i) if one knows d_k for $k=0,1,\ldots,n$, one can compute Δ by $\delta_k=d_k/d_{k-1}$ (without the need to find U, V explicitly); (ii) as representative of equivalence classes of matrices, the factors d_k are intrinsic characteristics of the relative orientation of the lattices, independent of the choice of a basis.

2. *The integral matrix*

If $T=A^{-1}B=(T_{ij})$ has rational entries we can write $T_{ij}=r_{ij}/s_{ij}$, where r_{ij} and s_{ij} are pairwise coprime for all $i,j=1,\ldots,n$ (the g.c.d. of r_{ij} and s_{ij} is 1). Let μ denote the least common multiple of all denominators s_{ij}; μ is the least positive integer such that μT is an integral matrix (it is simply the common denominator of the fractions r_{ij}/s_{ij}, as would be used in evaluating their sum). Then $\mu T=P$ is a matrix with integral entries

$$P_{ij}=\mu r_{ij}/s_{ij}. \tag{III.1}$$

It is straightforward to check that μ is invariant under right and left multiplication of T by modular matrices U and V: if $T'=UTV$, let μ' be the least positive integer such that $\mu'T'$ is integral; since μT is integral, $\mu T'$ is also integral, which proves that $\mu'\le\mu$; conversely, since $\mu'T'$ is integral, $\mu'T=\mu'U^{-1}T'V^{-1}$ is also integral, which proves that $\mu'\ge\mu$, and so finally $\mu'=\mu$.

Furthermore, if L_a and L_b have the same density, the greatest common divisor of all integers P_{ij} is equal to 1: indeed, if d divides all P_{ij} then d^n divides $\det(P)=\mu^n$; consequently, d divides μ but, after $r_{ij}/s_{ij}=(P_{ij}/d)/(\mu/d)$, the integer μ/d is a common multiple of all the denominators s_{ij}; this finally implies $d=1$ by definition of μ. Incidentally, this property, $\text{g.c.d.}(\{P_{ij}\})=1$, also holds under the weaker condition that $\det(P)$ does not contain any factor to the nth power.

In the above example, $\mu=5$ and therefore

$$P=\begin{bmatrix}4 & -3\\ 3 & 4\end{bmatrix}. \tag{III.2}$$

We can now apply Smith's decomposition to P, that is $P=U\Delta V^{-1}$, where U and V are modular and Δ is diagonal with integer entries $\delta_1,\ldots,\delta_n$ such that δ_k divides δ_{k+1} for $k=1,\ldots,n-1$. The transition matrix is then

$$T = A^{-1}B = \mu^{-1}U\Delta V^{-1}. \qquad \text{(III.3)}$$

Since U and V are modular matrices, they merely correspond to changes of bases in the respective lattices: $L_a = AU\mathbf{Z}^n$ and $L_b = BV\mathbf{Z}^n$. This amounts to defining new structure matrices $A' = AU$ and $B' = BV$ and a corresponding transition matrix $T' = A'^{-1}B'$ given by

$$A'^{-1}B' = \mu^{-1}\Delta. \qquad \text{(III.4)}$$

This matrix is, of course, still rational. The changes of bases are explicitly given by

$$\mathbf{a}'_i = AU\mathbf{e}_i = \sum_j U_{ji}\mathbf{a}_j, \qquad \mathbf{b}'_i = BV\mathbf{e}_i = \sum_j V_{ji}\mathbf{b}_j \qquad \text{(III.5)}$$

and these new bases are related by the elementary relations

$$\mathbf{b}'_i = (\delta_i/\mu)\mathbf{a}'_i. \qquad \text{(III.6)}$$

Thus the Smith decomposition of the transition matrix yields bases of L_a and L_b related by simple scalings, different in each direction.

In the previous example the Smith decomposition $P = U\Delta V^{-1}$ is provided by

$$U = \begin{bmatrix} 4 & 1 \\ 3 & 1 \end{bmatrix}, \qquad \Delta = \begin{bmatrix} 1 & 0 \\ 0 & 25 \end{bmatrix}, \qquad V = \begin{bmatrix} 1 & 7 \\ 0 & 1 \end{bmatrix}. \qquad \text{(III.7)}$$

The adapted bases ($\mathbf{a}'$) of L_a and ($\mathbf{b}'$) of L_b are given by $\mathbf{a}'_1 = 4\mathbf{a}_1 + 3\mathbf{a}_2$, $\mathbf{a}'_2 = \mathbf{a}_1 + \mathbf{a}_2$ and $\mathbf{b}'_1 = \mathbf{b}_1$, $\mathbf{b}'_2 = 7\mathbf{b}_1 + \mathbf{b}_2$. The corresponding diagonal transition matrix gives (see Fig. 1)

$$\mathbf{b}'_1 = \tfrac{1}{5}\mathbf{a}'_1, \qquad \mathbf{b}'_2 = 5\mathbf{a}'_2.$$

IV. Intersection and sum lattices in $\mathbf{R}^n$

The Smith normal form provides 'proportional' bases ($\mathbf{a}'$) and ($\mathbf{b}'$) of L_a and L_b for which the transition matrix is diagonal with rational entries. In this case, for each $i = 1, \ldots, n$, we have $p_i\mathbf{a}'_i = q_i\mathbf{b}'_i$ with integral p_i and q_i (provided by $p_i/q_i = \delta_i/\mu$). Dividing this equality by l.c.m.(p_i, q_i) we define $\varepsilon_i = [p_i/\text{l.c.m.}(p_i, q_i)]\mathbf{a}'_i = [q_i/\text{l.c.m.}(p_i, q_i)]\mathbf{b}'_i$. Then the one-dimensional lattices $\mathbf{Z}\mathbf{a}'_i$ and $\mathbf{Z}\mathbf{b}'_i$ are respectively $\alpha_i\mathbf{Z}\varepsilon_i$ and $\beta_i\mathbf{Z}\varepsilon_i$, where $\alpha_i = \text{l.c.m.}(p_i, q_i)/p_i$ and $\beta_i = \text{l.c.m.}(p_i, q_i)/q_i$ are both integers. Their intersection and sum are obtained as in one dimension (see § II.2). Finally, the intersection lattice $L_a \cap L_b$ and the sum lattice $L_a + L_b$ result as the direct sum of the one-dimensional components.

The intersection lattice (CSL)

For each value of the index i we have to compute the intersection of $\mathbf{Z}\mathbf{a}'_i$ with $\mathbf{Z}\mathbf{b}'_i$. Taking advantage of the rational relation $\delta_i\mathbf{a}'_i = \mu\mathbf{b}'_i$, it is straightforward to show that this intersection is spanned by the vector

$$[\delta_i/\text{g.c.d.}(\mu, \delta_i)]\mathbf{a}'_i = [\mu/\text{g.c.d.}(\mu, \delta_i)]\mathbf{b}'_i, \qquad \text{(IV.1)}$$

where g.c.d.(μ, δ_i) is the greatest common divisor of μ and δ_i. Now let us define M and N as the diagonal matrices with integer entries:

$$M_{ii} = \delta_i/\text{g.c.d.}(\mu, \delta_i) \qquad \text{and} \qquad N_{ii} = \mu/\text{g.c.d.}(\mu, \delta_i).$$

Since $M_{ii}\mathbf{a}'_i = N_{ii}\mathbf{b}'_i$ for all $i = 1, \ldots, n$, we have $A'M = B'N$. The intersection lattice is given by

$$L_a \cap L_b = A'M\mathbf{Z}^n = B'N\mathbf{Z}^n. \qquad \text{(IV.2)}$$

The corresponding structure matrix is therefore equal to $A'M = B'N = AUM = BVN$. The index of the intersection lattice with respect to L_a or L_b is given by

$$\begin{aligned}\text{index}\,[L_a \cap L_b, L_a] &= \text{index}\,[L_a \cap L_b, L_b] \\ &= |\det(M)| = |\det(N)| \\ &= \mu^n / \prod_{i=1}^{n} \text{g.c.d.}(\mu, \delta_i). \qquad \text{(IV.3)}\end{aligned}$$

In the example the intersection lattice $L_a \cap L_b$ is generated by $\mathbf{a}'_1 = 5\mathbf{b}'_1$ and $5\mathbf{a}'_2 = \mathbf{b}'_2$. In terms of the initial basis we have $\mathbf{a}'_1 = (4, 3)$ and $5\mathbf{a}'_2 = (5, 5)$. Using elementary operations, we can obtain a simpler basis of $L_a \cap L_b$ given by $\{(2, -1), (1, 2)\}$.

The sum lattice (DSC lattice)

The computation of the sum is also straightforward: for each $i = 1, \ldots, n$, we have merely to compute the sum of the one-dimensional lattices $\mathbf{Z}\mathbf{a}'_i$ and $\mathbf{Z}\mathbf{b}'_i$. Due to the rational relation between $\mathbf{a}'_i$ and $\mathbf{b}'_i$, any vector in this sum is of the form

$$k\mathbf{a}'_i + l\mathbf{b}'_i = [(k\mu + l\delta_i)/\mu]\mathbf{a}'_i = [(k\mu + l\delta_i)/\delta_i]\mathbf{b}'_i.$$

Since the numerators of these fractions are all multiples of g.c.d.(μ, δ_i), the sum lattice is spanned by the vector

$$[\text{g.c.d.}(\mu, \delta_i)/\mu]\mathbf{a}'_i = [\text{g.c.d.}(\mu, \delta_i)/\delta_i]\mathbf{b}'_i. \qquad \text{(IV.4)}$$

This vector is related to the M and N matrices introduced in the preceding section,

$$(N_{ii})^{-1}\mathbf{a}'_i = (M_{ii})^{-1}\mathbf{b}'_i.$$

The sum lattice $L_a + L_b$ is therefore given by

$$L_a + L_b = A'N^{-1}\mathbf{Z}^n = B^nM^{-1}\mathbf{Z}^n. \qquad \text{(IV.5)}$$

This identity provides the structure matrix of the sum lattice as $A'N^{-1} = B'M^{-1} = AUN^{-1} = BVM^{-1}$. The indices of either L_a or L_b with respect to the sum lattice are equal and given by

$$\begin{aligned}\text{index}\,[L_a, L_a + L_b] &= \text{index}\,[L_b, L_a + L_b] = |\det(M)| \\ &= |\det(N)| \\ &= \mu^n \Big/ \prod_{i=1}^{n} \text{g.c.d.}(\mu, \delta_i). \qquad \text{(IV.6)}\end{aligned}$$

Comparing with (IV.3), we can define the index Σ to be any of the indices appearing in (IV.3) or (IV.6). All these equations are summarized in

$$\Sigma = \mu^n \Big/ \prod_{i=1}^{n} \text{g.c.d.}(\mu, \delta_i). \qquad \text{(IV.7)}$$

There are situations where $\Sigma = \mu$, but this identity is not true in general (see the example in § VI.3 below). Equation (IV.7) always holds. In the above example the sum lattice $L_a \cap L_b$ is generated by $\frac{1}{5}\mathbf{a}'_1 = \mathbf{b}'_1$ and $\mathbf{a}'_2 = \frac{1}{5}\mathbf{b}'_2$. Using the initial basis we have $\frac{1}{5}\mathbf{a}'_1 = \frac{1}{5}(4, 3)$ and $\mathbf{a}'_2 = (1, 1)$.

V. Decomposition of the transition into shear transformations

1. *The two-dimensional case*

In this section we show that if two lattices L_a and L_b of the two-dimensional plane have the same density, any rational transition matrix relating them is equivalent to a simple rational shear transformation that can be computed algorithmically. In the previous section we saw that L_a and L_b have structure matrices $A' = AU$ and $B' = BV$ such that the corresponding transition matrix $T' = A'^{-1}B' = \mu^{-1}\Delta$ is rational and diagonal. Let δ_1 and δ_2 denote the diagonal entries of Δ. By the definition of μ, the equal density requirement implies that $\delta_1 = \text{g.c.d.}(\{P_{ij}\}) = 1$ (see § III.2) and consequently $\delta_2 = \mu^2$. Thus Δ is the diagonal integral matrix:

$$\Delta = \mu A'^{-1}B' = \begin{bmatrix} 1 & 0 \\ 0 & \mu^2 \end{bmatrix}. \qquad \text{(V.1)}$$

Our purpose is to find new structure matrices $A'' = A'U'$ and $B'' = B'V'$ such that the corresponding transition matrix $A''^{-1}B''$ is a simple shear matrix S. The general form of a rational shear matrix is $S = I + (m/p)|s\rangle\langle\sigma|$, using Dirac's bracket notations; $|s\rangle$ and $\langle\sigma|$ are the irreducible lattice vector and reciprocal vector respectively and m, p are integers. S has unit determinant if and only if $\langle\sigma|s\rangle = 0$, a condition that is assumed from now on. The action of S is given by

$$S|x\rangle = |x\rangle + (m/p)\langle\sigma|x\rangle|s\rangle. \qquad \text{(V.2)}$$

This transformation acts in the space of indices. By applying modular transformations, we can always assume that $s = \mathbf{e}_1$ and $\sigma = \mathbf{e}_2$. Consequently, we shall consider shear matrices of the form

$$S = I + (m/p)|\mathbf{e}_1\rangle\langle\mathbf{e}_2| = \begin{bmatrix} 1 & m/p \\ 0 & 1 \end{bmatrix}. \qquad \text{(V.3)}$$

For two lattices to be related by such a shear transformation means that the equivalence class of transition matrices contains one of the specified form

$$S = U'^{-1}(\mu^{-1}\Delta)V'. \qquad \text{(V.4)}$$

Putting these together, we must find the modular matrices U' and V' by solving

$$\begin{bmatrix} 1 & m/p \\ 0 & 1 \end{bmatrix} = \mu^{-1}U'^{-1}\begin{bmatrix} 1 & 0 \\ 0 & \mu^2 \end{bmatrix}V'. \qquad \text{(V.5)}$$

Multiplying this equation by μ shows that p must divide μ; conversely, multiplying the equation by p shows that μ must divide p: therefore we have $p = \mu$, which yields

$$\begin{bmatrix} \mu & m \\ 0 & \mu \end{bmatrix} = U'^{-1}\begin{bmatrix} 1 & 0 \\ 0 & \mu^2 \end{bmatrix}V'. \qquad \text{(V.6)}$$

Thus the left-hand side of (V.6) has therefore the same Smith normal form Δ as $A^{-1}B$. Obviously, m can be chosen in the interval $(-\mu/2, \mu/2)$ since other values correspond to right multiplication by convenient modular matrices. Consequently, the only condition on m is that g.c.d.$(m, \mu) = 1$, *i.e.* m and μ must be coprime (for instance, $m = 1$). Thus several shear matrices can be equivalent to $\mu^{-1}\Delta$, which means that a variety of different shear transformations actually map L_a onto L_b.

In any case, the modular factor in $S = U'^{-1}(\mu^{-1}\Delta)V'$ induce corresponding structure matrices $A'' = A'U'$ and $B'' = B'V'$ such that

$$S = A''^{-1}B'' = \begin{bmatrix} 1 & m/\mu \\ 0 & 1 \end{bmatrix}. \qquad \text{(V.7)}$$

Let $(\mathbf{a}'')$ and $(\mathbf{b}'')$ denote the corresponding basis of L_a and L_b. The above relation is then

$$\mathbf{b}''_1 = \mathbf{a}''_1, \qquad \mathbf{b}''_2 = \mathbf{a}''_2 + (m/\mu)\mathbf{a}''_1. \qquad \text{(V.8)}$$

The shear direction is given by the lattice vector $A''\mathbf{e}_1 = A'U'\mathbf{e}_1 = \mathbf{a}''_1$ and the shear invariant subspace is the line generated by the same vector $\mathbf{a}''_1$.

Remark. As already noticed, several equivalent shears map L_a onto L_b. Although the Smith form Δ of μS is unique, the modular matrices U' and V' are not uniquely defined. There exist pairs of modular matrices, P and Q, such that $P^{-1}\Delta Q = \Delta$. Since Δ is regular, this equation is equivalent to $Q = \Delta^{-1}P\Delta$ so that Q is uniquely determined by P. Thus we can define the group $H(\Delta)$ associated with Δ as the set of modular matrices P such that $Q(P) = \Delta^{-1}P\Delta$ has integer entries. This is a subgroup of the modular group GL$(2, \mathbf{Z})$. As a consequence, for each P in $H(\Delta)$, we have as well

$$S = U'^{-1}P^{-1}(\mu^{-1}\Delta)QV'.$$

In terms of the new structure matrices $A'' = A'PU'$ and $B'' = B'QV'$, we still have $S = A''^{-1}B''$, but the geometry might be different because it is referred to a different basis: for example, the shear direction is now $A''\mathbf{e}_1 = A'PU'\mathbf{e}_1$. In practice, it is convenient to choose (P, Q) so that the components of the vectors are small.

In the example of the $\mu = 5$ geometry, we have

$$A' = AU = \begin{bmatrix} 4 & 1 \\ 3 & 1 \end{bmatrix} \text{ and } \Delta = \begin{bmatrix} 1 & 0 \\ 0 & 25 \end{bmatrix}.$$

The shear matrices are of the form

$$S = \begin{bmatrix} 1 & m/5 \\ 0 & 1 \end{bmatrix}, \tag{V.9}$$

where m is coprime to 5. The matrix P must satisfy

$$\begin{bmatrix} 1 & 0 \\ 0 & 1/25 \end{bmatrix} P \begin{bmatrix} 1 & 0 \\ 0 & 25 \end{bmatrix} \in \mathrm{GL}(2, \mathbf{Z}). \tag{V.10}$$

We give the most simple solutions obtained for $m = -2$, -1 and 1.

(i) $m = -2$. The Smith decomposition $5S = U'^{-1}\Delta V'$ is

$$\begin{bmatrix} 5 & -2 \\ 2 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 25 \end{bmatrix} \begin{bmatrix} 5 & -2 \\ -2 & 1 \end{bmatrix}.$$

For $P = \begin{bmatrix} -6 & -1 \\ 25 & 4 \end{bmatrix}$,

$$A'' = A'PU' = \begin{bmatrix} 1 & 0 \\ -3 & 1 \end{bmatrix}.$$

The three-dimensional invariant plane of this shear is of type (3, 1, 0) and corresponds to a known mirror plane of the $\Sigma = 5$ grain boundaries. However, for

$$P = \begin{bmatrix} -7 & -2 \\ 25 & 7 \end{bmatrix}, \quad A'' = \begin{bmatrix} 7 & -1 \\ -6 & 1 \end{bmatrix}$$

and the invariant plane (670) is not a mirror plane.

(ii) $m = -1$. The Smith decomposition is

$$5S = \begin{bmatrix} 5 & -1 \\ 0 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -5 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 25 \end{bmatrix} \begin{bmatrix} 5 & -1 \\ 1 & 0 \end{bmatrix}.$$

Setting P equal to the identity matrix, we get

$$A'' = A'PU' = \begin{bmatrix} 9 & 1 \\ 8 & 1 \end{bmatrix}.$$

(iii) $m = 1$. The Smith decomposition is now

$$5S = \begin{bmatrix} 5 & 1 \\ 0 & 5 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 5 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 25 \end{bmatrix} \begin{bmatrix} 5 & 1 \\ -1 & 0 \end{bmatrix}.$$

For $P = \begin{bmatrix} -7 & -1 \\ 50 & 7 \end{bmatrix}$, $A'' = \begin{bmatrix} 7 & 3 \\ 9 & 4 \end{bmatrix}$; but for $P = \begin{bmatrix} -6 & -1 \\ 25 & 4 \end{bmatrix}$, $A'' = \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix}$.

Notice that, in all cases, the first column of the A'' matrix is a vector of the CSL. The invariant plane that is perpendicular to this vector sometimes is, and sometimes is not, a mirror plane, according to the choice of the shear vector, in (i) and (iii) each possibility is displayed.

2. *The general n-dimensional case*

We assume that L_a and L_b have the same density, which implies that the determinant of the transition matrices is equal to ± 1. The adapted bases ($\mathbf{a}'$) and ($\mathbf{b}'$) defined in § III yield a rational and diagonal transition matrix $T' = \mu^{-1}\Delta$ and we have the relation $\mu^n = \delta_1 \ldots \delta_n$. We show in this section that L_a and L_b can be related by at most $n-1$ elementary shear transformations. Moreover, each shear transformation has a lattice direction, a rational amplitude and an invariant plane with integral Miller indices. The proof relies on a recursive procedure, depending on the dimension n, and a simple lemma relative to 2×2 integral matrices, extending the result of the previous section.

Lemma. Let Δ be a 2×2 diagonal integral matrix with entries δ_1 and δ_2. Assume that there is an integer μ such that δ_1 divides μ and μ divides δ_2. Then there exist modular matrices U and V such that $\mathcal{T} = U\Delta V$ is an upper triangular matrix with diagonal entries $\mathcal{T}_{11} = \delta_1\delta_2/\mu$ and $\mathcal{T}_{22} = \mu$.

Proof. Possible solutions for U and V are provided by the identity

$$\begin{bmatrix} 1 & 0 \\ \mu/\delta_1 & 1 \end{bmatrix} \begin{bmatrix} \delta_1 & 0 \\ 0 & \delta_2 \end{bmatrix} \begin{bmatrix} \delta_2/\mu & 1 \\ -1 & 0 \end{bmatrix} = \begin{bmatrix} \delta_1\delta_2/\mu & \delta_1 \\ 0 & \mu \end{bmatrix}, \tag{V.11}$$

since μ/δ_1 and δ_2/μ are integers.

We can now state the following theorem.

Theorem. Let Δ denote a diagonal integral $n\times n$ matrix with positive entries $\delta_1, \ldots, \delta_n$. Assume that δ_1 divides δ_2, $\ldots$, δ_{n-1} divides δ_n and that $\delta_1\delta_2 \ldots \delta_n = \mu^n$ for some integer μ. Then there exist integral modular $n\times n$ matrices U and V such that $\mathcal{T} = U\Delta V$ is an integral upper triangular matrix with diagonal entries $\mathcal{T}_{ii} = \mu$ for $i = 1, \ldots, n$.

Proof. The proof proceeds by induction on the dimension n of the matrices. The result is obvious for $n = 1$ and the above lemma gives the proof for $n = 2$ since $\delta_1\delta_2 = \mu^2$. Assume the result is true up to dimension $n-1$ and consider an $n\times n$ matrix Δ satisfying the assumptions of the theorem. Since the sequence of diagonal entries is increasing, δ_1 divides μ and μ divides δ_n. Use the above lemma to get a new matrix with μ as the (n, n) entry

$$\begin{bmatrix} 1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 \\ \mu/\delta_1 & 0 & \ldots & 0 & 1 \end{bmatrix} \begin{bmatrix} \delta_1 & 0 & \ldots & 0 & 0 \\ 0 & \delta_2 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & \delta_{n-1} & 0 \\ 0 & 0 & \ldots & 0 & \delta_n \end{bmatrix}$$

$$\times \begin{bmatrix} \delta_n/\mu & 0 & \ldots & 0 & 1 \\ 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 \\ -1 & 0 & \ldots & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} \delta_1\delta_n/\mu & 0 & \ldots & 0 & \delta_1 \\ 0 & \delta_2 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & \delta_{n-1} & 0 \\ 0 & 0 & \ldots & 0 & \mu \end{bmatrix}$$

$$= \begin{bmatrix} D_{n-1} & & \delta_1 \\ & & \vdots \\ 0 & \ldots & \mu \end{bmatrix}. \tag{V.12}$$

Denote by U'' and V'' the left and right modular multiplies of Δ on the first line of this equation.

Now the submatrix D_{n-1} consisting of the first $(n-1)$ rows and the first $(n-1)$ columns is diagonal and integral. D_{n-1} is not necessarily in the Smith form but there exist $(n-1)\times(n-1)$ modular matrices U_{n-1} and V_{n-1} such that $U_{n-1}D_{n-1}V_{n-1}=\Delta_{n-1}$ is its Smith normal form. The product of the diagonal entries of Δ_{n-1} is $\det(\Delta_{n-1})=\det(D_{n-1})=\mu^{n-1}$; by the recurrence hypothesis there exist $(n-1)\times(n-1)$ modular matrices U' and V' such that $U'\Delta_{n-1}V'=\mathcal{T}_{n-1}$ is an upper triangular matrix with diagonal entries equal to μ. Finally,

$$\begin{bmatrix} U' & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} U_{n-1} & 0 \\ 0 & 1 \end{bmatrix} U''\Delta V'' \begin{bmatrix} V_{n-1} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} V' & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \mu & * & \ldots & * & * \\ 0 & \mu & \ldots & * & * \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & \mu & * \\ 0 & 0 & \ldots & 0 & \mu \end{bmatrix}, \tag{V.13}$$

where $*$ denotes an unspecified entry. This completes the proof.

The decomposition of a rational transition matrix into $n-1$ rational shears is now straightforward.

(1) The transition matrix is $T=A^{-1}B=\mu^{-1}U\Delta V^{-1}$, where Δ is the Smith normal form of μT.

(2) For some modular matrices U' and V', $U'\Delta V'=\mathcal{T}$ is an upper triangular matrix with diagonal entries equal to μ; the diagonal matrix Δ is therefore equivalent to $\mathcal{T}$ and there exist structure matrices A'' and B'' such that $A''^{-1}B''=\mu^{-1}\mathcal{T}$.

(3) The modular upper triangular matrix $\mu^{-1}\mathcal{T}$ is the product of $n-1$ rational shear matrices.

The last point is a consequence of the fact that any triangular matrix M with diagonal entries 1 is equal to a product of $n-1$ shear matrices: $M=S_{n-1}\ldots S_2S_1$. For $k=1,\ldots,n$, S_k is the identity matrix except for the kth row, which is equal to that of M.

$$S_k = \begin{bmatrix} 1 & 0 & \ldots & \ldots & \ldots & 0 \\ 0 & \ddots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \ldots & 1 & M_{k,k+1} & \ldots & M_{k,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & \ldots & \ldots & \ldots & 0 & 1 \end{bmatrix}. \tag{V.14}$$

In our case, $S_k=I+|e_k\rangle\langle\sigma_k|$ where e_k is the kth vector of the standard basis and σ_k is the covector defined by $\langle\sigma_k|e_i\rangle=\mu^{-1}\mathcal{T}_{ki}$ for $i\neq k$ and $\langle\sigma_k|e_k\rangle=0$.

VI. Applications in three dimensions

In three dimensions the diagonal transition matrix reads $T'=\mu^{-1}\Delta$, where

$$\Delta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \delta_2 & 0 \\ 0 & 0 & \delta_3 \end{bmatrix}. \tag{VI.1}$$

The coefficients satisfy $\mu^3=\delta_2\delta_3$ and δ_2 divides δ_3. Notice that, in distinction to two dimensions where it was uniquely determined by μ, the Smith matrix can take different forms in $n\geq 3$ dimensions, according to the possible ways of factorizing μ^n. We will characterize some in this section.

We start with a classical result that can be recovered in a straightforward way by means of the Smith decomposition.

1. *Cubic lattices*

Assume L_a and L_b are cubic and that the structure matrices A and B are such that $T=A^{-1}B$ is a rotation with rational entries. T satisfies $T^tT=I$ (the superscript t denotes the transposed matrix) and, as a consequence, $P=\mu T$ satisfies $P^tP=\mu^2 I$; the comatrix $\tilde{P}$ of P satisfies $P^t\tilde{P}=\det(P)I=\mu^3 I$, which implies $\tilde{P}=\mu P$. Now the factor $d_2=\delta_1\delta_2=\delta_2$ is the g.c.d. of all the 2×2 minors of P; since these minors are (up to a sign) the entries of $\tilde{P}$ we conclude that $\delta_2=\text{g.c.d.}(\{\tilde{P}_{ij}\})=\mu\times\text{g.c.d.}(\{P_{ij}\})=\mu$. Finally, $\delta_3=\mu^2$ and the diagonal transition matrix is necessarily

$$\Delta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \mu^2 \end{bmatrix}. \tag{VI.2}$$

Then g.c.d.$(\mu, \delta_i) = \mu$ for $i = 2, 3$ and formula (IV.7) for the index yields $\Sigma = \mu$, a result proved by Grimmer *et al.* (1974) with an involved proof.

It follows from the general results of § V that L_a can always be mapped onto L_b by two successive rational shears. The conditions under which the transition can be performed by a single shear are now given.

2. *The single-shear case*

In this case, structural matrices $A'' = A'U'$ and $B'' = B'V'$ can be found such that

$$A''^{-1}B'' = S = \begin{bmatrix} 1 & m/p & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = U'^{-1}(\mu^{-1}\Delta)V',$$

where m and p are coprime integers. As in the two-dimensional case, multiplying this equation by μ or p shows that $p = \mu$. Therefore Δ is the Smith form of the integral matrix

$$\mu S = \begin{bmatrix} \mu & m & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \mu \end{bmatrix} = U'^{-1} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \delta_2 & 0 \\ 0 & 0 & \delta_3 \end{bmatrix} B'.$$

Comparison of the elementary divisors of both sides yields: (i) m and μ are coprime and (ii) δ_2 is the g.c.d. of μm and μ^2. This implies $\delta_2 = \mu$ and $\delta_3 = \mu^2$. Conversely, if the matrix Δ has diagonal entries 1, μ and μ^2, Δ is equivalent to μS with m coprime to μ. Thus, this situation is completely characterized by Δ being of the form (VI.2). From (IV.7) we see that the index Σ is equal to μ.

As a corollary, the expression (VI.2) for the Δ matrix in the case where cubic lattices correspond to each other by a pure rotation (without distortion) shows that the rotation is indeed equivalent to a single shear. This feature of rational rotations is very different from the general irrational ones where as many as four shears are generally necessary (Duneau & Oguey, 1991).

3. *The double-shear case*

As an example, we may define the structure matrices A and B as

$$A = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad B = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 4 \end{bmatrix}.$$

The transition matrix T is then

$$T = A^{-1}B = \tfrac{1}{2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 8 \end{bmatrix}.$$

Therefore $\mu = 2$ (albeit $\Sigma = 4$ in this case) and the Smith form of $2T$ is the diagonal matrix Δ with entries 1, 1 and 8. Δ is equivalent to the matrix $2S$, where

$$S = \begin{bmatrix} 1 & \frac{1}{2} & 0 \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & \frac{1}{2} & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

is clearly a product of two simple shears and the Smith decomposition is $2S = U^{-1}\Delta V$:

$$2S = \begin{bmatrix} 2 & 1 & 0 \\ 0 & 2 & 1 \\ 0 & 0 & 2 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & 2 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 8 \end{bmatrix}\begin{bmatrix} 2 & 1 & 0 \\ -4 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}.$$

The adapted bases of L_a and L_b are given by the structure matrices

$$A' = AU = \begin{bmatrix} 2 & 0 & 0 \\ -4 & 2 & 0 \\ 4 & -2 & 1 \end{bmatrix}, \qquad B' = BV = \begin{bmatrix} 2 & 1 & 0 \\ -4 & 0 & 1 \\ 4 & 0 & 0 \end{bmatrix}.$$

Then $A'^{-1}B' = S$ and the corresponding bases ($\mathbf{a}'$) and ($\mathbf{b}'$), given by the columns of A' and B', satisfy the relations

$$\mathbf{b}'_1 = \mathbf{a}'_1, \qquad \mathbf{b}'_2 = \mathbf{a}'_2 + \tfrac{1}{2}\mathbf{a}'_1, \qquad \mathbf{b}'_3 = \mathbf{a}'_3 + \tfrac{1}{2}\mathbf{a}'_2.$$

4. *An example in the hexagonal system*

The geometry of twins in the hexagonal system is more complicated than in the cubic system. The standard basis of a hexagonal Bravais lattice L_a is given by the three-dimensional structure matrix

$$A = \begin{bmatrix} a & a/2 & 0 \\ 0 & a3^{1/2}/2 & 0 \\ 0 & 0 & c \end{bmatrix}. \tag{VI.3}$$

If $B = RA$ is the structure matrix of L_b, the corresponding transition matrix is given by

$$T = A^{-1}B = A^{-1}RA.$$

The condition for the existence of a CSL (or a DSCL) is that T has rational entries. We shall focus on the following solution, which, among others, was recently examined by Hagège (1991). The geometrical parameters are the following:

(1) c/a has the value $(\frac{7}{2})^{1/2}$.

(2) the rotation R is specified by the rotation axis [0100] and the angle $\theta \simeq 85.59°$, for which $\cos\theta = \frac{1}{13}$ and $\sin\theta = (\frac{12}{13})(\frac{7}{6})^{1/2}$.

The two-dimensional lattice $L_a \cap P$, where the plane P is perpendicular to the rotation axis, is spanned by the vectors $\alpha_1=[10\bar{1}0]$, of length $a3^{1/2}$, and $\alpha_2=[0001]$, of length c. In this plane the two-dimensional structure matrix A_P of $L_a \cap P$ is

$$A_P=\begin{bmatrix} a3^{1/2} & 0 \\ 0 & c \end{bmatrix}.$$

Thus $\alpha_1=A_P\mathbf{e}_1$ and $\alpha_2=A_P\mathbf{e}_2$ where $(\mathbf{e}_1,\mathbf{e}_2)$ is the standard basis of the two-dimensional plane. Since $B_P=RA_P$, the two-dimensional transition matrix $T=A_P^{-1}B_P$ is easily computed from the above data,

$$T=\tfrac{1}{13}\begin{bmatrix} 1 & -14 \\ 12 & 1 \end{bmatrix}. \tag{VI.4}$$

Similarly, $L_b \cap P$ is spanned by $\beta_1=B_P\mathbf{e}_1$ and $\beta_2=B_P\mathbf{e}_2$.

Of course, $\mu=13$ and the Smith decomposition of $\mu T=U\Delta V^{-1}$ is

$$\mu T=\begin{bmatrix} 1 & -14 \\ 12 & 1 \end{bmatrix}=\begin{bmatrix} 1 & 0 \\ 12 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 169 \end{bmatrix}\begin{bmatrix} 1 & -14 \\ 0 & 1 \end{bmatrix}.$$

The proportional bases of L_a and L_b in P are given by the structure matrices $A'_P=A_PU$ and $B'_P=B_PV$: we have $\alpha'_1=\alpha_1+12\alpha_2$, $\alpha'_2=\alpha_2$ and $\beta'_1=\beta_1$, $\beta'_2=14\beta_1+\beta_2$. The relationship between these two bases is given by:

$$\beta'_1=\alpha'_1/13,$$
$$\beta'_2=13\alpha'_2.$$

The intersection lattice $L_a \cap L_b$ in P is spanned by $(\alpha'_1, 13\alpha'_2)$, while the sum lattice L_a+L_b is spanned by $(\alpha'_1/13, \alpha'_2)$.

The relative orientation relationship can be described by a shear transformation associated with the shear matrix S,

$$S=\begin{bmatrix} 1 & \frac{1}{13} \\ 0 & 1 \end{bmatrix}. \tag{VI.5}$$

The Smith decomposition of the integral matrix $\mu S=U'^{-1}\Delta V'$ is

$$\mu S=\begin{bmatrix} 13 & 1 \\ 0 & 13 \end{bmatrix}=\begin{bmatrix} 1 & 0 \\ 13 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 169 \end{bmatrix}\begin{bmatrix} 13 & 1 \\ -1 & 0 \end{bmatrix}.$$

The structure matrices $A''=A'U'$ and $B''=B'V'$ give rise to the new basis

$$\alpha''_1=\alpha'_1-13\alpha'_2=\alpha_1-\alpha_2,$$
$$\alpha''_2=\alpha'_2=\alpha_2,$$
$$\beta''_1=13\beta'_1-\beta'_2=-\beta_1-\beta_2,$$
$$\beta''_2=\beta'_1=\beta_1,$$

in which the shear transformation is described by

$$\beta''_1=\alpha''_1, \qquad \beta''_2=\alpha''_2+\alpha'_1/13.$$

The shear direction is given by $\alpha''_1=\alpha_1-\alpha_2=[10\bar{1}\bar{1}]$. Since the axis of the rotation is spanned by $[0100]$, the invariant plane of the shear transformation is given by $(10\bar{1}2)$, which is the twinning plane of the $\Sigma=13$ hexagonal system (Hagège, 1991).

VII. Concluding remarks

The shear decomposition of transition matrices between lattices of equal density seems to be a convenient procedure to classify the relative orientations. In generic situations, four shears are required and we believe that particular cases where only one or two shears are sufficient are of physical interest. This is actually the case when the lattices and their relative orientation give rise to coincidence lattices and rational transition matrices. The shears involved in such transitions have the further advantage that their invariant planes provide natural candidates for the interface planes. The shear decompositions of the transition matrices between pairs of lattices are easily obtained by means of the theory of Smith normal forms. We have seen that the double-shear condition is fulfilled in all cases where a coincidence lattice exists, whatever the symmetry of the lattices.

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