

N-Dimensional Coincidence-Site-Lattice Theory

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Abstract

A matricial theory of coincidence-site and displacement-shift-complete (DSC) lattices of arbitrary dimension is developed. Vector bases for these lattices can easily be determined from particular factorizations of the matrix defining the relative orientation. Various properties of the two lattices are derived, including the reciprocity relations. The general conditions for coincidence and the problem of coincidence in sublattices of lower dimension are also discussed.

1. Introduction

Coincidence-site-lattice (CSL) theory has deserved considerable attention in recent years, mostly as a consequence of the relative success of the models of crystalline interfaces based on the properties of CSL and related lattices (Brandon, Ralph, Ranganathan & Wald, 1964; Bollmann, 1970; Pumphrey, 1976). Most of the work has been on CSL's of two identical three-dimensional lattices, especially cubic lattices (Ranganathan, 1966; Fortes, 1972; Grimmer, 1973; Grimmer, Bollmann & Warrington, 1974; Bleris & Delavignette, 1981) and hexagonal lattices (Fortes, 1973; Warrington, 1975; Bonnet, Cousineau & Warrington, 1981), although attention has also been given to the general case of two different three-dimensional lattices (Bucksch, 1972; Santoro & Mighell, 1973; Grimmer, 1976; Iwasaki, 1976; Bonnet & Cousineau, 1977; Fortes, 1977; Bacmann, 1979). These lattices are, of course, of special importance in solid-state physics and metallurgy, but recently attention has been given to lattices of higher dimension (*e.g.* by Schwarzenberger, 1974; Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978).

Both matrix algebra and number theory are fundamental tools in the study of CSL's and both have been used to derive a considerable number of properties and methods of analysis of such lattices. In some cases, however, properties have been enunciated without satisfactory proof, and, in general, rather different methods of derivation were used by different authors to

establish them. The purpose of this paper is therefore to present a unified, formal theory of CS and related lattices and to précis some of the literature results. The theory is applicable to any two *n*-dimensional lattices. The study of coincidence between two lattices of different dimensions, *m* and *n* (*m* < *n*), can always be reduced to that case, by considering the sublattice of the *n*-dimensional lattice that lies in the space spanned by the *m*-dimensional lattice. However, we shall treat explicitly coincidence in sublattices of lower dimension than the dimension of the two given lattices. The theory is first presented for the case where a CSL can be defined of the same dimension as that of the given lattices. The problem of coincidence in sublattices of lower dimension will be discussed in § 5.

2. General formulation

2.1. Sublattices and superlattices

Consider an *s*-dimensional lattice with a vector basis $(\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_s) = (\mathbf{e})$. The lattice vectors are of the form $\sum_i a_i \mathbf{e}_i$, where the a_i can take any integral values independently of each other. The metric matrix $G = (g_{ij})$ is defined by $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$. The volume of the primitive cell defined by (\mathbf{e}) is

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

For three-dimensional lattices it is frequently important to determine the type of Bravais lattice; this can be done from G using the method of reduced cells.

Consider a second set of *s* vectors (\mathbf{e}') related to the (\mathbf{e}) by a non-singular (square) matrix $U = (u_{ij})$ of order *s*:

$$[\mathbf{e}'_1 \mathbf{e}'_2 \dots \mathbf{e}'_s] = [\mathbf{e}_1 \mathbf{e}_2 \dots \mathbf{e}_s] U, \quad (2)$$

where $[\mathbf{e}_1 \dots \mathbf{e}_s]$, for example, is to be regarded as a row matrix and the product (2) is calculated according to the rules of matrix algebra:

$$\mathbf{e}'_i = \sum_j \mathbf{e}_j u_{ji}. \quad (3)$$

Since U is non-singular, the set (\mathbf{e}') defines another s -dimensional lattice, the metric matrix of which is

$$G' = U^T G U, \quad (4)$$

where U^T is the transpose of U . A condensed notation $\mathbf{e} = [\mathbf{e}_1 \dots \mathbf{e}_s]$ will be used in matricial equations. Equation (2) is then written as

$$\mathbf{e}' = \mathbf{e} U \quad (5a)$$

or

$$\mathbf{e} = \mathbf{e}' U^{-1}. \quad (5b)$$

Three particular cases will be considered (*cf.* Santoro & Mighell, 1972):

1. $U = T$ is an integral matrix (i matrix) with $\det T = 1$ (which we call a 1 matrix). The lattice defined by (\mathbf{e}') is identical to lattice (\mathbf{e}) since all vectors of the former are vectors of the latter and *vice versa* (note that T^{-1} is also a 1 matrix). The matrix T just defines a change of basis, *i.e.* the two sets of vectors are two different bases of the same lattice.

2. $U = N$ is an i matrix with $|\det N| = \Sigma$. The vectors (\mathbf{e}') belong to the lattice (\mathbf{e}) and define a sublattice of (\mathbf{e}) . Since $\det G' = \Sigma^2 \det G$, it can be concluded from (1) that the volume of a primitive cell of the sublattice is Σ times the volume of the cell of lattice (\mathbf{e}) , that is, $\Omega' = \Sigma \Omega$.

3. $U = M^{-1}$, where M is an i matrix with $|\det M| = \Sigma'$. In this case $\mathbf{e} = \mathbf{e}' M$ and (\mathbf{e}) is a sublattice of (\mathbf{e}') . The basis (\mathbf{e}') then defines a superlattice of (\mathbf{e}) , *i.e.* a lattice that contains (\mathbf{e}) . The relation between the volumes of primitive cells is Σ' , that is, $\Omega' = \Omega / \Sigma'$.

There is a fourth important case in which U is a rational matrix (r matrix). This case will now be discussed in detail.

2.2. Coincidence-site lattice; degree of coincidence

Consider two s -dimensional lattices with bases (\mathbf{e}) and (\mathbf{e}') . One may think that the two lattices interpenetrate in an s -dimensional Euclidean space. Then there is a relation of type (2) between the two bases, the matrix U defining the relative orientation of the two lattices. It will be assumed that the two lattices have one lattice point in common; this is always possible if a convenient translation is given to one of the lattices. The conditions under which the two lattices contain a common sublattice of dimension s will now be investigated. In this case, the two lattices have coincident points which form an s -dimensional lattice.

The vector bases of sublattices of (\mathbf{e}) and (\mathbf{e}') , respectively, have the general form $\mathbf{e}N$ and $\mathbf{e}'N'$, where N and N' are any i matrices (*cf.* § 2.1). Therefore, for a common sublattice to exist, it is necessary that there are two i matrices, N and N' , such that

$$\mathbf{e} N = \mathbf{e}' N' \quad (6a)$$

or

$$\mathbf{e} = \mathbf{e}' N' N^{-1}. \quad (6b)$$

The matrix $U \equiv X$ which relates the two bases must then be of the form

$$X = N' N^{-1}; \mathbf{e} = \mathbf{e}' X. \quad (7)$$

Since N^{-1} is in general an r matrix (because $N^{-1} = \text{adj } N / \det N$, where $\text{adj } N$ is an i matrix and $\det N$ is an integer) one may conclude that a common sublattice of dimension s implies that X be rational. Conversely, if the matrix X relating the two bases is rational, it can always be written in the form (7). In fact, if n is the smallest integer such that nX is an i matrix, it is enough to take for N a diagonal matrix with all diagonal elements equal to n . This is the general condition for coincidence, as already enunciated by Grimmer (1976) for three-dimensional lattices: a common sublattice of dimension s exists if and only if the matrix X relating the two bases is an r matrix. Alternative conditions for coincidence in two- and three-dimensional lattices were formulated by Bucksch (1972), which cannot easily be generalized for n -dimensional lattices.

When X is rational, the CSL is defined as the sublattice that contains all points in coincidence. It is therefore the common sublattice which has a primitive cell of smallest volume. All common sublattices are sublattices of the CSL. To determine this lattice, one has to find a factorization of X of the type

$$X = N' N^{-1}, \quad (8)$$

with the smallest possible values of $|\det N|$ and $|\det N'|$. These values will be denoted by Σ and Σ' . They indicate the reciprocal fraction of coincidence points (or *degree of coincidence*) in lattices (\mathbf{e}) and (\mathbf{e}') , respectively. A factorization of X with the smallest absolute values Σ , Σ' of the determinants of the integral-factor matrices will be termed a *c factorization*. Then, if N and N' are c cofactors of X , the basis of the CSL is

$$\mathbf{e}N = \mathbf{e}'N'. \quad (9)$$

An equivalent c factorization is one with factors NS , $N'S$, where S is an arbitrary 1 matrix.

In the following various methods for determining Σ and Σ' for a given X (r matrix) will be indicated. The derivation of the first two methods is given in the preceding paper (Fortes, 1983). We write X in the form $X = (t/q)Q$, where t and q are coprime integers and Q is an i matrix with elements that do not admit a common divisor: then q is the smallest positive integer such that qX is an i matrix. We find a set of s positive numbers d_i for the matrix Q , termed the invariant set, such that d_i is the greatest common divisor (GCD) of all square submatrices of Q of order i . Clearly $d_1 = 1$

and $d_s = |\det Q|$. Then we determine s numbers q_i (the elementary divisors of Q):

$$\begin{aligned} q_1 &= d_1 \\ q_i &= d_i/d_{i-1}. \end{aligned} \quad (10)$$

A diagonal matrix with elements q_i is equivalent to Q . As shown in the preceding paper, the general method for obtaining the degree of coincidence is:

Method 1. The degree of coincidence in lattice (\mathbf{e}) is given by

$$\Sigma = q_{(1)} \dots q_{(s)}$$

with

$$q_{(i)} = \frac{q}{\text{GCD}(q, q_i)}.$$

After finding Σ we may obtain $\Sigma' = \Sigma |\det X|$.

Alternative methods can be formulated to determine Σ and Σ' , by using the matrices X and X^{-1} . We indicate here only the methods for matrices of order 3; q' is the smallest integer such that $q' X^{-1}$ is an i matrix. Then (Fortes, 1983)

Method 2. For three-dimensional lattices, Σ is the smallest positive integer such that

$$\frac{\Sigma}{q} \quad \text{and} \quad \frac{\Sigma \det X}{q'}$$

are integers. Σ' is the smallest positive integer such that

$$\frac{\Sigma'}{q'} \quad \text{and} \quad \frac{\Sigma'}{q \det X}$$

are integers. Σ and Σ' are also the smallest positive integers such that

$$\frac{\Sigma}{q} \quad \text{and} \quad \frac{\Sigma'}{q'}$$

are integers and $\Sigma'/\Sigma = |\det X|$.

An equivalent method that follows immediately is

Method 3. For three-dimensional lattices, Σ is the smallest positive integer such that ΣX and $(\Sigma \det X)X^{-1}$ are i matrices and $\Sigma \det X$ is an integer. $\Sigma' = \Sigma |\det X|$ is the smallest positive integer such that $\Sigma' X^{-1}$ and $(\Sigma'/\det X)X$ are i matrices and $\Sigma'/\det X$ is an integer.

The first two conditions determining Σ and Σ' expressed in method 3 have already been enunciated by Grimmer (1976). However, it is in general necessary to add the last condition, namely, that $\Sigma \det X$ (or $\Sigma'/\det X$) must be an integer. An example with $X = \frac{1}{2}I$, where I is the identity matrix, shows that the first two conditions are not sufficient to determine Σ and Σ' . The conditions expressed in method 2 are, at any rate, simpler than those in method 3. Alternative methods for determining the degree of coincidence in two- and

three-dimensional lattices have been developed by Bucksch (1972).

The main results of this section can be summarized in the following points:

1. A CSL exists if and only if the orientation matrix X is rational.

2. The basis of the CSL is $\mathbf{e}N = \mathbf{e}' N'$, where N and N' are c cofactors of X .

3. The degree of coincidence can be obtained by method 1 (or method 2 or 3 for three-dimensional lattices).

2.3. DSC lattice

A superlattice of (\mathbf{e}) is defined by $\mathbf{e}M^{-1}$, where M is an arbitrary i matrix. Two lattices (\mathbf{e}) and (\mathbf{e}') have a common superlattice if there are i matrices M, M' such that

$$\mathbf{e}M^{-1} = \mathbf{e}'M'^{-1} \quad (11a)$$

or

$$\mathbf{e} = \mathbf{e}'M'^{-1}M = \mathbf{e}'X. \quad (11b)$$

The matrix X relating the two lattices has to be an r matrix of the form

$$X = M'^{-1}M. \quad (12)$$

Conversely, if X is rational it can be written in the form (12) and there is a common superlattice. When X is rational, the DSC (displacement-shift-complete) lattice is defined as the coarsest superlattice, *i.e.* the superlattice with the largest volume of a primitive cell. All common superlattices are superlattices of the DSCL. The DSCL can also be defined as the coarsest lattice that contains all vectors of the form $\mathbf{v} + \mathbf{v}'$, where \mathbf{v}, \mathbf{v}' are vectors of (\mathbf{e}) and (\mathbf{e}') , respectively (Bollmann, 1970).

For a given X , the DSCL is determined by making a factorization of type (12) with the smallest possible values of $|\det M|, |\det M'|$. Such a factorization will be termed a d factorization. Noting that $X^T = M^T(M'^T)^{-1}$, a d factorization of X can be obtained from a c factorization of X^T , because transposition does not change the invariants d_i . The values Σ, Σ' defined previously are therefore the minimum values of $|\det M'|$ and $|\det M|$ respectively, *i.e.* the two factorizations are defined by

$$X = N'N^{-1}; \quad \Sigma = |\det N|; \quad \Sigma' = |\det N'|$$

$$X = M'^{-1}M; \quad \Sigma = |\det M'|; \quad \Sigma' = |\det M| \quad (13)$$

with Σ, Σ' given by any of the methods indicated above.

A basis of the DSC lattice is

$$\mathbf{e}M^{-1} = \mathbf{e}' M'^{-1}, \quad (14)$$

which defines a cell with a volume $1/\Sigma'$ times the volume of the cell (\mathbf{e}) and a volume $1/\Sigma$ times the volume of the cell (\mathbf{e}').

The vectors of the DSCL have components (h_1, \dots, h_s) in the basis (\mathbf{e}) which are the solutions of

$$M\{h\} = \{i\}. \quad (15)$$

The symbol $\{ \}$ indicates a column vector: $\{i\}$ is a column vector with integral elements. It is easily shown that the h_i are of the form $h_i = p_i/\Sigma'$, where the p_i are the integral solutions of

$$\frac{M}{\Sigma'} \{p\} = \{i\}. \quad (16)$$

The DSCL vectors have rational components of the form α/β (α, β coprime), where β is among the divisors of $\Sigma' = \det M$.

2.4. Determination of c and d factorizations

The actual determination of c and d factorizations relies on the determination of integral solutions of linear equations with rational (integral) coefficients. For third-order matrices, Grimmer (1977), following Bonnet (1976), has given an algorithm to determine both factorizations, which in fact relies on the solution of diophantine equations. In general, one of the factors can be taken as a triangular matrix. This is a consequence of the possibility of choosing a basis of a lattice (in the present case the CSL or DSCL) with the successive vectors in particular sublattices (of increasing dimension) of the lattice. Grimmer's algorithm can easily be generalized to n -dimensional lattices (Grimmer, 1981).

3. Reciprocity relations

The reciprocity relations between the CSL and DSCL were first derived by Grimmer (1974a) for three-dimensional lattices using essentially number theory. More recently, the same relations were derived for space lattices by Iwasaki (1976) using group theory and by Bacmann (1979) using Poisson distributions. The following derivation for n -dimensional lattices is based on matrix algebra.

As shown in § 2 if

$$\mathbf{e} = \mathbf{e}'X \quad (17)$$

with X rational, the two lattices (\mathbf{e}) and (\mathbf{e}') (of the same dimension) have a CSL and a DSCL (of the same dimension as the original lattices), the bases of which are defined by the matrices obtained in c and d factorizations of X . Denoting by G and G' the metric matrices of the two lattices, and by G_C and G_D the metric matrices of the CSL and DSCL, one may write

$$G = X^T G' X$$

$$G_C = N^T G N$$

$$G_D = (M^{-1})^T G M^{-1} \quad (18)$$

Equivalent expressions for G_C and G_D could be written with the matrices N', M', G' .

The reciprocal basis (\mathbf{r}) of any lattice (\mathbf{e}) is defined as

$$\mathbf{r} = \mathbf{e}G^{-1} \quad (19)$$

Combining (17)–(19) one obtains the well-known relation

$$\mathbf{r} = \mathbf{r}'(X^T)^{-1}. \quad (20)$$

The reciprocal lattices are also related by an r matrix, the c and d factorizations of which are easily related to those of X . For example,

$$(X^T)^{-1} = [M^T(M'^{-1})^T]^{-1} = M'^T(M^T)^{-1}, \quad (21)$$

which is a c factorization of $(X^T)^{-1}$.

Bases of the various lattices and reciprocal lattices can now be determined with the following results:

CSL of reciprocal lattices:

$$\mathbf{r}M^T = \mathbf{e}G^{-1}M^T;$$

DSCL of reciprocal lattices:

$$\mathbf{r}(N^T)^{-1} = \mathbf{e}G^{-1}(N^T)^{-1};$$

reciprocal lattice of CSL:

$$\mathbf{e}N(N^T G N)^{-1} = \mathbf{e}G^{-1}(N^T)^{-1};$$

reciprocal lattice of DSCL:

$$\mathbf{e}M^{-1}[(M^{-1})^T G M^{-1}]^{-1} = \mathbf{e}G^{-1} M^T.$$

These relations show that the CSL (DSCL) of the reciprocal lattices is the reciprocal lattice of the DSCL (CSL) of the two lattices.

4. Determination of coincidence orientations

Given two s -dimensional lattices defined by their metric matrices G and G' (or by their bases), an important problem is to find the relative orientations for which a CSL (and therefore a DSCL) exists. A CSL orientation $\mathbf{e} = \mathbf{e}'X$ is defined by any r matrix X , such that

$$G = X^T G' X. \quad (22)$$

Attempts at finding the general solution of this equation were made by Santoro & Mighell (1973) and by Bonnet & Cousineau (1977); and special methods were developed for two identical cubic lattices (Grimmer, 1974b; Bleris & Delavignette, 1981) and hexagonal lattices (Bonnet *et al.*, 1981).

In the following discussion, it will be assumed that a particular rational solution X_0 of this equation has been

determined. Of course, the existence of a solution implies some restrictions on G and G' (Bucksch, 1972; Fortes, 1977) and in general (22) will be impossible with X rational.

If a particular solution X_0 has been found, all the other rational solutions X can be obtained from X_0 by multiplication by the rational rotation matrices of one of the lattices. Such matrices, for lattice G , are the (rational) solutions of

$$R^T G R = G. \quad (23)$$

More precisely, the general rational solution of (22) is

$$X = X_0 R, \quad (24)$$

where R is the general (rational) solution of (23) and X_0 is a particular solution of (22). These results follow immediately from an analysis of (22) and (23). It is also possible to obtain the general solution using the rotation matrices R' of (\mathbf{e}'):

$$X = R' X_0. \quad (25)$$

For the same solution X , the two matrices R and R' in (24) and (25) are related by $R' = X_0 R X_0^{-1}$. The traces of R and R' are therefore the same, this meaning that the 'angles of rotation' (which are related to the trace, t , by $t = 2 \cos \theta + s - 2$) are θ and $-\theta$. It can also be shown that the $(s - 1)$ -dimensional sublattice of (\mathbf{e}) that remains invariant in the rotation R (e.g. the rotation axis in three-dimensional lattices) is in coincidence with the corresponding (\mathbf{e}') sublattice for R' . All these results are of simple interpretation, noting that what matters is the relative rotation away from the CSL orientation defined by X_0 .

In conclusion, if one CSL orientation is known all the others can be obtained by rotating one of the lattices away from that orientation, the rotation being a CSL rotation of that particular lattice. A more subtle conclusion is the following: if a CSL orientation exists, the two lattices will admit CSL rotations of the same angle in a one-to-one correspondence.

5. Coincidence in sublattices of lower dimension

So far we have discussed a particular type of coincidence between two s -dimensional lattices, namely, the one in which the coincident points define an s -dimensional CSL. For this case we have indicated methods of determining the fraction of coincident points, that is the ratio between the volume of the cell of the CSL and that of each of the original lattices. We have also studied the properties of the DSC lattice and its relation to the CSL. We shall treat in this section the possibility of coincidence in sublattices of dimension $r < s$, which may of course occur even if there is not an s -dimensional CSL.

5.1. Definitions

The term r sublattice will be used to designate a sublattice of lower dimension, r , of a given lattice. A CSL in an r sublattice will accordingly be termed an r CSL.

Any r sublattice of a lattice (\mathbf{e}) may be defined by a $s \times r$ rectangular i matrix C , of rank r . The basis of the r sublattice is the set of r independent vectors.

$$\mathbf{e}C. \quad (26)$$

This r sublattice will be termed a complete r sublattice (cr sublattice) if it contains all vectors of (\mathbf{e}) that are parallel to any vector of the r sublattice. It is easy to show that in this case the matrix C must have the following property: the equation $CD^{-1} = i$ matrix only admits solutions in D (an i matrix $r \times r$) with $|\det D| = 1$. By a sublattice of the cr sublattice C we shall mean an r sublattice of C with the same dimension. Any such r sublattice has a basis of the type

$$\mathbf{e}CN, \quad (27)$$

where N is an $r \times r$ i matrix.

The degree of coincidence in an r sublattice (complete or not) is the reciprocal fraction of coincident points in that r sublattice relative to all points in the same sublattice. The complete degree of coincidence is defined in relation to the cr sublattice.

5.2. Conditions for coincidence in r sublattices

Consider again two lattices (\mathbf{e}) and (\mathbf{e}'), of the same dimension s , related by a matrix X ,

$$\mathbf{e} = \mathbf{e}' X. \quad (28)$$

A vector $\mathbf{h}_1 = \sum_i h_i \mathbf{e}_i$ of lattice (\mathbf{e}) (the h_i are integers) is a *coincident vector* if and only if there is an equal vector in lattice (\mathbf{e}'), that is, if

$$X \{h_1\} = \{i\}, \quad (29)$$

where $\{h_1\}$ is a column matrix and $\{i\}$ is an arbitrary integral column matrix. If it is possible to find r such vectors (and no more than r) that are linearly independent, there is coincidence in an r sublattice of (\mathbf{e}) (but not in sublattices of higher dimension). A basis of that r sublattice is defined by the set of r vectors ($\mathbf{h}_1, \mathbf{h}_2, \dots, \mathbf{h}_r$), or equivalently by a rectangular $r \times s$ matrix C , the columns of which are the components of each of the \mathbf{h}_i ; the basis is $\mathbf{e}C$. For an r CSL to exist in the r sublattice C of lattice (\mathbf{e}), it is necessary and sufficient that an i matrix N ($r \times r$) can be found such that

$$XC N = \{i\}. \quad (30)$$

In fact, in this case

$$\mathbf{e}C N = \mathbf{e}' X C N = \mathbf{e}' \{i\} \quad (31)$$

and vectors of the r sublattice C coincide with vectors of (\mathbf{e}') . The degree of coincidence Σ is of course the smallest value of $|\det N|$ for N satisfying (30). With this N , a basis for the r CSL is defined by (31). Note that the complete degree of coincidence is $p\Sigma$, where $p = |\det D|$, D being a matrix with largest p such that $CD^{-1} = i$ matrix. If we had considered an r sublattice C' of (\mathbf{e}') , the condition for coincidence would be

$$X^{-1}C'N' = \{i\} \quad (32)$$

and the degree of coincidence, Σ' , the smallest value of $|\det N'|$ with N' satisfying (32). The complete degree of coincidence is $p'\Sigma'$. The actual determination of Σ , Σ' will not be dealt with in detail.

Clearly, conditions (30) or (32) do not imply that X be an r matrix. If it is, the two lattices are in a CSL orientation, coincidence occurs in all r sublattices, and (30) or (32) have solutions N , N' for any integral rectangular matrices C , C' .

To end this section, we shall find the general form of X for which coincidence in r sublattices occurs. As discussed above, given two lattices (\mathbf{e}) and (\mathbf{e}') of dimension s , coincidence will occur in an r sublattice, if it is possible to find two $s \times r$ integral i matrices C , C' such that

$$\mathbf{e}C = \mathbf{e}'C'. \quad (33)$$

The above vectors define a basis of the r CSL of that r sublattice (we assume that C , C' are of rank r). We now construct extended matrices C_{ex} and C'_{ex} obtained from C and C' by adding $(s - r)$ columns of real numbers, with a first restriction that C_{ex} and C'_{ex} should be non-singular. Then

$$\mathbf{e}C_{\text{ex}} = \mathbf{e}'C'_{\text{ex}} \quad (34)$$

or

$$\mathbf{e} = \mathbf{e}'X; \quad X = C'_{\text{ex}}C_{\text{ex}}^{-1} \quad (35)$$

defines a relative orientation for which coincidence in the r sublattices C and C' occurs. Note that the relation $G = X^T G' X$, where G and G' are given matrices, imposes further restrictions on the real numbers used to extend C and C' . Clearly X does not have to be rational.

5.3. Degree of coincidence in $(s - 1)$ sublattices

As shown in the preceding paper (Fortes, 1983), the maximum coincidence in complete r sublattices of (\mathbf{e}) corresponds to a degree of coincidence equal to the invariant divisor d_r [cf. § 2.2 and equation (10)] of the matrix N in a c factorization of the orientation matrix X .

It will now be assumed that the two lattices of dimension s are in a CSL orientation. We shall discuss in detail the method of determining the degree of coincidence in sublattices of dimension $s - 1$. This

problem is particularly important in the context of crystalline interfaces, where it is frequently of interest to know the degree of coincidence in the planes of two space lattices in a CSL orientation. An $(s - 1)$ sublattice is more conveniently defined by a vector $\mathbf{v} = \sum \mathbf{r}_i v_i$, of the reciprocal lattice, which is perpendicular to all vectors of the sublattice. The two representations are related by

$$\{v\}^T C = 0, \quad (36)$$

where C is an $s \times (s - 1)$ matrix defining the $(s - 1)$ sublattice and $\{v\}^T$ is a row vector with elements v_i . If C defines a complete sublattice, the v_i should be taken as coprime integers; we shall consider only this case. The corresponding vector \mathbf{v}' of the reciprocal lattice (\mathbf{r}') is obtained from

$$\{v'\} = (X^{-1})^T \{v\}. \quad (37)$$

Let Σ be the degree of coincidence of the two lattices, referred to lattice (\mathbf{e}) and N the corresponding c cofactor of X . The complete degree of coincidence Σ_c in the (complete) sublattice of (\mathbf{e}) defined by C or \mathbf{v} is determined as follows. Let q be the largest positive integer such that

$$(1/q) \sum_i v_i \mathbf{r}_i \quad (38)$$

is a vector of the reciprocal lattice of the CSL. A basis (\mathbf{R}) of this reciprocal lattice is [see end of § 2 and equation (19)]

$$\mathbf{R} = \mathbf{r}(N^T)^{-1}. \quad (39)$$

If the vector (38) is a vector of lattice (\mathbf{R}) then

$$(1/q) N^T \{v\} = \{i\}. \quad (40)$$

Since N is known, the largest positive integer q can be determined from this equation for each \mathbf{v} . There is one in every q sublattices \mathbf{v} where coincidence occurs, a consequence of the way q was defined. The degree of coincidence Σ_c in the sublattice is then

$$\Sigma_c = \Sigma/q. \quad (41)$$

The $(s - 1)$ sublattices can be classified according to the values of Σ_c , which are necessarily divisors of Σ and multiples of the invariant d_{s-1} of the matrix N . One may also find the $(s - 1)$ sublattices which correspond to a particular value of Σ_c . To do this, consider the lattices with bases \mathbf{r} and $\mathbf{r}(N^T/q)$. The vectors \mathbf{v} which are solutions of (40) are the vectors of the CSL of these two lattices. A basis for this CSL can be found in the usual way, by determining a c factorization of N^T/q :

$$N^T/q = P'P^{-1}. \quad (42)$$

The sublattices for each value of q have normals \mathbf{v} which are lattice vectors of the CSL $\mathbf{r}P$. They are then of the form

$$\{v\}^T = P\{i\}^T. \quad (43)$$

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References

- BACMANN, J.-J. (1979). *Acta Cryst.* **A35**, 553–563.
 BLERIS, G. L. & DELAVIGNETTE, P. (1981). *Acta Cryst.* **A37**, 779–786.
 BOLLMANN, W. (1970). *Crystal Defects and Crystalline Interfaces*. Berlin: Springer.
 BONNET, R. (1976). *Scr. Metall.* **10**, 801–803.
 BONNET, R. & COUSINEAU, E. (1977). *Acta Cryst.* **A33**, 850–856.
 BONNET, R., COUSINEAU, E. & WARRINGTON, D. H. (1981). *Acta Cryst.* **A37**, 184–189.
 BRANDON, D. G., RALPH, B., RANGANATHAN, S. & WALD, M. S. (1964). *Acta Metall.* **12**, 813–821.
 BROWN, H., BÜLOW, R., NEUBÜSER, J., WONDRATSCHEK, H. & ZASSENHAUS, H. (1978). *Crystallographic Groups of Four-Dimensional Space*. New York: Wiley.
 BUCKSCH, R. (1972). *J. Appl. Cryst.* **5**, 96–102.
 FORTES, M. A. (1972). *Rev. Fis. Quim. Eng. Ser. A*, **4**, 7–17.
 FORTES, M. A. (1973). *Scr. Metall.* **7**, 821–823.
 FORTES, M. A. (1977). *Phys. Status Solidi B*, **82**, 377–382.
 FORTES, M. A. (1983). *Acta Cryst.* **A39**, 348–350.
 GRIMMER, H. (1973). *Scr. Metall.* **7**, 1295–1300.
 GRIMMER, H. (1974a). *Scr. Metall.* **8**, 1221–1224.
 GRIMMER, H. (1974b). *Acta Cryst.* **A30**, 685–688.
 GRIMMER, H. (1976). *Acta Cryst.* **A32**, 783–785.
 GRIMMER, H. (1977). *Ber. Herbsttagung Schweiz. Phys. Ges.* **50**, 141–142.
 GRIMMER, H. (1981). Private communication.
 GRIMMER, H., BOLLMANN, W. & WARRINGTON, D. H. (1974). *Acta Cryst.* **A30**, 197–207.
 IWASAKI, Y. (1976). *Acta Cryst.* **A32**, 59–65.
 PUMPHREY, P. H. (1976). *Grain Boundary Structure and Properties*, edited by G. A. CHADWICK & D. A. SMITH, ch. 5. New York: Academic Press.
 RANGANATHAN, S. (1966). *Acta Cryst.* **21**, 197–199.
 SANTORO, A. & MIGHELL, A. D. (1972). *Acta Cryst.* **A28**, 284–287.
 SANTORO, A. & MIGHELL, A. D. (1973). *Acta Cryst.* **A29**, 169–175.
 SCHWARZENBERGER, R. L. E. (1974). *Proc. Cambridge Philos. Soc.* **76**, 23–32.
 WARRINGTON, D. H. (1975). *J. Phys.* **36** (Suppl. to No. 10) c4-98-95.

Acta Cryst. (1983). **A39**, 357–368

Point-Group Determination by Convergent-Beam Electron Diffraction

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Abstract

The method of point-group determination from convergent-beam electron diffraction patterns has been established by Buxton, Eades, Steeds & Rackham [*Philos. Trans. R. Soc. London* (1976), **281**, 171–194]. However, Table 2 given by them is inconvenient for practical purposes, since many symmetries of the dark-field and $\pm G$ dark-field patterns are not given and are left for the reader's consideration. The table is improved and completed with the help of some new symmetry symbols and illustration of symmetries. The new table makes the point-group determination easy and quick. The symmetries of the symmetrical many-beam convergent-beam electron diffraction patterns have been studied by Tinnappel [PhD Thesis (1975), Tech. Univ. Berlin] using group theory. It is shown that the graphical method used by Buxton *et al.* can reveal the symmetries of these patterns. A method of

point-group determination which uses three types of symmetrical many-beam patterns, the hexagonal six-beam, square four-beam and rectangular four-beam patterns, is described. This method requires only one photograph in determining most diffraction groups. This fact means that the method is more convenient and reliable than that of Buxton *et al.*, since their method requires two or three photographs for most cases. Experimental results which verify the theoretical ones are given. The characteristic features of the symmetrical many-beam method are discussed.

Introduction

The recent crystallographic studies by means of convergent-beam electron diffraction (CBED) originated with Goodman & Lehmpfuhl (1965), although the earlier work by Kossel & Möllenstedt (1939) was done about four decades ago. They obtained CBED patterns by converging a conical electron beam of an angle of more than 10^{-2} rad on a small area of a

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