J. Appl. Cryst. (1973). **6**, 400

The Construction of Orthogonal Supercells of an Arbitrary Lattice

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(*Received* 1 *March* 1973; *accepted* 6 *April* 1973)

A lattice is called orthogonal if it possesses at least monoclinic symmetry. Necessary and sufficient conditions for the existence of orthogonal supercells of a given arbitrary lattice and procedures for calculating them are presented. In addition the conditions for the existence of supercells of higher symmetry, especially cubic and hexagonal, are discussed. Applications to the following crystallographic problems are suggested: geometrical twinning conditions, coincidence-site lattices, conventional supercells of primitive cells, criteria whether a given zonal net can belong to a tetragonal or hexagonal lattice, derivation of possible structural relationships of a lattice to such of higher symmetries from the geometry of the unit cell prior to the knowledge of the structure.

1. Introduction

The crystallographer often asks for lattice rows which are perpendicular or approximately perpendicular to a lattice plane. This problem is of interest, for instance, in the geometrical theory of twinning. Moreover the question may arise whether a given lattice possesses a subcell or a supercell of higher symmetry, especially cubic or hexagonal. The existence of such subcells or supercells may provide valuable clues for the solution of structures and for certain relationships among different structure types. The problem of orthogonal supercells has already been treated by Niggli (1928) and by other crystallographers, especially von Lang (1896) and Brezina (1884), but a general method of solution is still missing. The perpendicularity conditions for triclinic and monoclinic lattices as presented in the *International Tables for X-ray Crystallography* (1959), for instance, are too restrictive.

In § 2 the necessary and sufficient conditions for the existence of a rectangular supermesh of a net will be derived. In addition the conditions for the existence of square and hexagonal supermeshes will be discussed. The analogous problem for the case of a space lattice will be treated in § 3 with special emphasis on the existence of cubic, hexagonal and tetragonal supercells. In § 4 certain practical applications to crystallographic problems will be discussed.

2. Rectangular supermeshes of a net

Let $\mathbf{a}_1$ and $\mathbf{a}_2$ be the basis vectors of a net. The vectors

$$\left.\begin{array}{l}\mathbf{r}_1=[u_1,v_1]=u_1\mathbf{a}_1+v_1\mathbf{a}_2\\ \text{and}\\ \mathbf{r}_2=[u_2,v_2]=u_2\mathbf{a}_1+v_2\mathbf{a}_2\end{array}\right\}\ u_i,v_i \text{ integer for } i=1,2 \quad (1)$$

are perpendicular to each other if and only if

$$\mathbf{r}_1\,.\,\mathbf{r}_2=u_1u_2s_{11}+v_1v_2s_{22}+(u_1v_2+u_2v_1)s_{12}=0\ , \quad (2)$$

with

$$s_{ij}=s_{ji}=\mathbf{a}_i\,.\,\mathbf{a}_j(i,j=1,2)\ . \quad (3)$$

The symmetrical matrix

$$\mathbf{S}=\{s_{ij}\} \quad (4)$$

is called the *metric tensor* of the mesh defined by the basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. Introducing the *mesh matrix*

$$\mathbf{M}=\begin{pmatrix}\mathbf{a}_1\\ \mathbf{a}_2\end{pmatrix}, \quad (5)$$

with the basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ in terms of Euclidean space as its rows, we may write

$$\mathbf{S}=\mathbf{M}\tilde{\mathbf{M}}\ , \quad (6)$$

where $\tilde{\mathbf{M}}$ is the transposed matrix of $\mathbf{M}$. The metric tensor $\mathbf{S}$ is independent of the special choice of the Euclidean axes. With

$$n_{11}=u_1u_2 \quad (7a)$$

$$n_{22}=v_1v_2 \quad (7b)$$

$$n_{12}=u_1v_2+u_2v_1 \quad (7c)$$

we may rewrite the perpendicularity condition (2) in the form

$$n_{11}s_{11}+n_{22}s_{22}+n_{12}s_{12}=0\ \ (n_{ij}\text{ integer})\ . \quad (8)$$

From the equations (7*a*–*c*) we obtain the following relation among the integers n_{ij}:

$$n_{12}^2-4n_{11}n_{22}=D^2, \quad (9)$$

with

$$D=u_1v_2-u_2v_1\ . \quad (10)$$

The existence of integers n_{11}, n_{22}, n_{12} and D satisfying equations (8) and (9) is not only necessary but also sufficient for the existence of a rectangular supermesh. Its edges $[u_1,v_1]$ and $[u_2,v_2]$ are obtained by the equations

$$2n_{11}:(n_{12}-D)=u_1:v_1 \tag{11}$$

$$2n_{11}:(n_{12}+D)=u_2:v_2\,. \tag{12}$$

If $n_{11}=0$, s_{11} and s_{22} are to be interchanged in condition (8). These equations are easily verified with the aid of the equations (7*a–c*) and (10). These results are summarized in the following basic theorem:

Theorem 1

A net with the metric tensor $\mathbf{S}=\{s_{ij}\}$ contains two mutually perpendicular vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ if and only if there exists a rational relationship $n_{11}s_{11}+n_{22}s_{22}+n_{12}s_{12}=0$ with integer coefficients n_{ij} among the elements s_{ij} of the metric tensor, such that $D^2=n_{12}^2-4n_{11}n_{22}$ is a squared integer. D is the index of the rectangular supermesh, defined by the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$.

The integers n_{ij} satisfying equation (8) can be found by a procedure due to Lagrange and introduced into crystallography by Johnsen & Toeplitz (1918). In this procedure the vectors (100), (010) and (001) are assigned to the elements s_{11}, s_{22} and s_{12} respectively, of the metric tensor S. By subtracting appropriate multiples of the smallest of these numbers from the remaining ones these are made as small as possible and corresponding vectors are assigned to them. To the number, say $s_{11}-3s_{12}$, the vector $(10\bar{3})$ is assigned. By repeating this procedure several times one arrives at last at a 'vector' $(n_{11},n_{22},n_{12})=\varepsilon\simeq 0$, which is just a brief symbol of equation (8). If there is more than one 'vector' (n_{11},n_{22},n_{12}) satisfying equation (8) within the range of errors one should try to find the vector with the smallest elements n_{ij} by linear combination of them, taking account of the residuals and ensuring that condition (9) is satisfied.

The existence of two different vectors $n_i=(n_{11}^i,n_{22}^i,n_{12}^i)$ $(i=1,2)$ satisfying condition (8) exactly implies that the elements s_{ij} of S have the ratio of integers.

If the coefficients s_{ij} of the metric tensor S have the ratio of reasonably small integers S_{ij} there exist many rectangular meshes with reasonably small index D. This case is conveniently treated by making use of the reciprocal lattice as will be shown now. Let $\mathbf{a}_1^*$ and $\mathbf{a}_2^*$ be the basis vectors of the reciprocal net. Then we have, by definition:

$$\mathbf{a}_i\,.\,\mathbf{a}_j^*=\delta_{ij}\,, \tag{13}$$

with

$$\delta_{ij}=\begin{cases}1, & \text{if } i=j\\ 0, & \text{if } i\neq j\,.\end{cases}$$

Let the vector

$$\mathbf{r}^*(h,k)=h\mathbf{a}_1^*+k\mathbf{a}_2^* \tag{14}$$

of the reciprocal net be parallel to the vector $\mathbf{r}(u,v)$ of the direct net, that is

$$u\mathbf{a}_1+v\mathbf{a}_2=\lambda(h\mathbf{a}_1^*+k\mathbf{a}_2^*)\,. \tag{15}$$

By scalar multiplication of this equation with the basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ we obtain, with the defining equations (3) and (13) in mind:

$$\begin{aligned}us_{11}+vs_{12}&=\lambda h\\ us_{12}+vs_{22}&=\lambda k\,.\end{aligned} \tag{16}$$

With the aid of the *covectors* $\mathbf{u}=[u,v]$ and $\mathbf{h}=(h,k)$ of the vectors $\mathbf{r}$ and $\mathbf{r}^*$ respectively, the linear equations (16) can briefly be written

$$\mathbf{Su}=\lambda\mathbf{h}\,, \tag{17}$$

with the vectors $\mathbf{u}$ and $\mathbf{h}$ written columnwise.

In the metric tensor S the elements s_{ij} should be replaced by the integers S_{ij} proportional to them. Then the parameter λ becomes an integer if $\mathbf{h}$ is to be a primitive vector. λ is always a divisor of the determinant of the integer metric tensor S, as will be proven later. The metric tensor $\mathbf{S}=\{S_{ij}\}$ with integer elements S_{ij} which have no common divisor $\neq 1$ is called a '*normalized*' metric tensor. Now the vector $[-k,h]$ of the direct net is perpendicular to the vector $\mathbf{h}=(h,k)$ of the reciprocal net. With the aid of the tensor equation (17) we find, therefore, at once the vector which is normal to any given vector $\mathbf{u}$ of the direct net.

The index D of the rectangular supermesh defined by $\mathbf{u}$ and $\mathbf{u}'=[-k,h]$ is equal to

$$D=\mathbf{u}\,.\,\mathbf{h}=\tilde{\mathbf{u}}\mathbf{h}\,, \tag{18}$$

where $\tilde{\mathbf{u}}$ is the vector $\mathbf{u}$ written as a row. Combining equations (17) and (18) we obtain

$$\tilde{\mathbf{u}}\mathbf{S}\mathbf{u}=\lambda\tilde{\mathbf{u}}\mathbf{h}=\lambda D\,. \tag{19}$$

The expression on the left-hand side of this equation is nothing else than the so-called quadratic form of the net, explicitly

$$u^2S_{11}+v^2S_{22}+2uvS_{12}=Q(u,v)=\lambda D \tag{20}$$

which provides the squares of the vectors $\mathbf{r}_i(u,v)$ of the normalized net defined by S. Before discussing the square and hexagonal supermeshes let me illustrate the results obtained by two numerical examples. Let

$$\mathbf{S}=\begin{pmatrix}7{\cdot}203 & 3{\cdot}126\\ 3{\cdot}126 & 17{\cdot}532\end{pmatrix}$$

be the metric tensor of a net. In the following scheme we derive the coefficients n_{ij} of condition (8) by the method of Johnsen & Toeplitz (1918). The upper three rows of this scheme contain the elements s_{11}, s_{22} and

s_{12}, the lower three rows the vectors assigned to them, in the same order:

$$\begin{array}{ccc} 7{\cdot}203 & 0{\cdot}951 & 0{\cdot}951 \\ 17{\cdot}532 & 1{\cdot}902 & \mathbf{0{\cdot}000} \\ 3{\cdot}126 & 3{\cdot}126 & 0{\cdot}273 \\[6pt] 100 & 10\bar{2} & 10\bar{2} \\ 010 & 01\bar{5} & \mathbf{\bar{2}1\bar{1}} \\ 001 & 001 & \bar{3}07\,. \end{array}$$

According to this calculation we have $n_{11}=-2$, $n_{22}=1$ and $n_{12}=-1$. These numbers satisfy condition (9) of Theorem 1 with $D=3$. We have, therefore, a threefold rectangular supermesh. The coordinates $[u_i, v_i]$ of its edges are obtained by equations (11) and (12):

$$u_1:v_1 = 1:1$$
$$u_2:v_2 = -2:1\,.$$

The metric tensor S of this supermesh with the edges $\mathbf{a}_1'=[1,1]$ and $\mathbf{a}_2'=[\bar{2},1]$ becomes.

$$\mathbf{S}'=\begin{pmatrix} 30{\cdot}987 & 0{\cdot}000 \\ 0{\cdot}000 & 33{\cdot}840 \end{pmatrix}.$$

Since in any rectangular net the vectors $[u,v]$ and $[u,\bar{v}]$ have the same length, the vectors $\mathbf{a}_1'+\mathbf{a}_2'=[\bar{1},2]$ and $\mathbf{a}_1'-\mathbf{a}_2'=[3,0]$ (in terms of the original net) are equally long. One could, therefore, establish the existence of a rectangular supermesh by finding two equally long vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ in a net, for then the vectors $\mathbf{r}_1+\mathbf{r}_2$ and $\mathbf{r}_1-\mathbf{r}_2$ define a rectangular supermesh. But this procedure is in general more laborious than our method. It can be of help, however, if there exists a computed list of point distances. In most practical cases condition (8) will not be satisfied as exactly as in our constructed example. The vector $(n_{11}n_{22}n_{12})=(\bar{3}07)$ of our example, for instance, which satisfies equation (8) only approximately, would be an acceptable solution for most purposes. This solution yields an approximately rectangular supermesh with the edges $\mathbf{a}_1''=[1,0]$ and $\mathbf{a}_2''=[3,7]$ and the metric tensor

$$\mathbf{S}''=\begin{pmatrix} 7{\cdot}203 & 0{\cdot}273 \\ 0{\cdot}237 & 792{\cdot}603 \end{pmatrix}.$$

The angle of this sevenfold supermesh differs from a right angle only by about 12 minutes of arc.

As an additional example let us consider a net with the metric tensor

$$\mathbf{S}=\begin{pmatrix} 4{\cdot}29 & 1{\cdot}43 \\ 1{\cdot}43 & 10{\cdot}01 \end{pmatrix}.$$

Its elements have the ratio $s_{11}:s_{22}:s_{12}=3:7:1$. We replace, therefore, this tensor by the normalized tensor

$$\mathbf{S}'=\begin{pmatrix} 3 & 1 \\ 1 & 7 \end{pmatrix}.$$

Table 1 lists the vectors $\mathbf{u}'=\left(\begin{smallmatrix}\bar{0}&1\\1&0\end{smallmatrix}\right)\mathbf{h}$ which are perpendicular to some preselected primitive vectors $\mathbf{u}$ according to equation (17), together with the values of the parameter λ, of the index $D=\mathbf{u}\,.\,\mathbf{h}$, and of $Q=\lambda D$.

Table 1. *Rectangular supermeshes derived from the numerical example*

No.	u	v	u'	v'	λ	D	Q
1	1	0	$\bar{1}$	3	1	3	3
2	0	1	$\bar{7}$	1	1	7	7
3	1	1	$\bar{2}$	1	4	3	12
4	1	$\bar{1}$	3	1	2	4	8
5	3	$\bar{2}$	11	7	1	43	43
6	2	1	$\bar{9}$	7	1	23	23
7	1	$\bar{2}$	13	1	1	27	27
8	$\bar{3}$	1	1	2	4	7	28

It should be noticed that the values of the parameters λ are divisors of the determinant of $\mathbf{S}'$, which in our case is equal to 20. That this is not only accidentally the case will be proven now. We formulate this statement in the following theorem:

Theorem 2

Let $\mathbf{u}=[u,v]$ (or $[u,v,w]$) be a primitive integer vector and let $\mathbf{S}$ be an integer 2×2 (or 3×3) matrix with the determinant S. Then the vector $\mathbf{h}=\mathbf{u}\mathbf{S}$ is either primitive or the λ-fold of a primitive vector, where λ is a divisor of S.

Proof: Since $\mathbf{u}$ is a primitive vector another vector $\mathbf{u}'$ (or two other vectors $\mathbf{u}'$ and $\mathbf{u}''$) can be found such that the determinant of the matrix

$$\mathbf{U}=\begin{pmatrix} u & v \\ u' & v' \end{pmatrix} \quad \text{or} \quad \mathbf{U}=\begin{pmatrix} u & v & w \\ u' & v' & w' \\ u'' & v'' & w'' \end{pmatrix}$$

is equal to 1. Then the determinant of the matrix $\mathbf{US}$ is equal to S. The first row of this matrix is the vector $\mathbf{h}$. If the elements of this vector have a common divisor λ, then λ is also a divisor of the determinant S of $\mathbf{US}$.

This theorem is valid for any number $n>1$ of dimensions. Also the equations (18) and (19) hold for the three-dimensional case if D is taken as the index of the monoclinic supercell defined by the vector $\mathbf{u}$ as its unique axis and the primitive mesh of the lattice plane defined by the rel-vector $\mathbf{h}$. Formula (20) then becomes

$$u^2S_{11}+v^2S_{22}+w^2S_{33}+2vwS_{23}+2uwS_{13} \\ +2uvS_{12}=Q(u,v,w)=\lambda D\,.$$

According to equations (17) and (20) the factor λ is contained in $Q(u,v)$. This must be borne in mind if one looks for all rectangular supermeshes with an index D not greater than a prefixed upper limit.

$$\mathbf{M}_1=\begin{pmatrix}u_1v_1\\u_2v_2\end{pmatrix}\begin{pmatrix}\mathbf{a}_1\\\mathbf{a}_2\end{pmatrix}=\mathbf{TM} \tag{21}$$

with

$$\mathbf{T}=\begin{pmatrix}u_1v_1\\u_2v_2\end{pmatrix}$$

is the mesh matrix of the supermesh defined by the vectors $[u_i,v_i]$. Its metric tensor $\mathbf{S}_1$ becomes [equation (6)]

$$\mathbf{S}_1=\mathbf{M}_1\tilde{\mathbf{M}}_1=\mathbf{TS}\tilde{\mathbf{T}}\ , \tag{22}$$

and consequently the determinant of this tensor becomes $|\mathbf{T}|^2\ .\ S=D^2S$. The determinant of the metric tensor of a mesh or a cell is also called the *discriminant* of the mesh or cell.

In the case of a rectangular supermesh of index D we have [equation (20)]

$$D^2S=Q(u_1,v_1)\ .\ Q(u_2,v_2)=\lambda_1\ .\ \lambda_2D^2, \tag{23}$$

from which follows

$$S=\lambda_1\ .\ \lambda_2\ . \tag{24}$$

In order to get the shorter edges of all rectangular supermeshes with an index $=D$ one has to consider only primitive vectors $[u_1,v_1]$ for which $Q(u_1,v_1)=\lambda D$, where λ is a divisor of S and $\leq\sqrt{S}$. Table 1 contains all rectangular supercells with an index $D\leq 7$.

A rectangular mesh has non-trivial rectangular supermeshes if and only if the squares of its edges have the ratio of integers. By a *trivial supermesh* is meant a mesh formed by multiples of the original edges.

We shall now prove the following theorem on the conditions for the existence of square supermeshes:

Theorem 3

A mesh possesses a square supermesh if and only if the elements s_{ij} of its metric tensor have the ratio of integers S_{ij} and if the determinant of the 'normalized' metric tensor $\mathbf{S}'=\{S_{ij})$ is a square number.

Proof: The necessary condition of an integer ratio of the elements s_{ij} follows from the fact that these have to satisfy the two conditions of equality and perpendicularity of the basis vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ of the square supermesh.

Because the discriminant $S_1'=D^2S'$ [equation (22)] of a square supermesh must obviously be a square number the same statement must apply to the discriminant S' of the original mesh.

Now it remains to be proven that any mesh satisfying these conditions does possess a square supermesh. Evidently the area of this supermesh, which is identical with the element S_{11}' of its metric tensor, must be a multiple of the (integer) square root of the determinant S' of $\mathbf{S}'$. (In the following we consider only normalized metric tensors.) We have, therefore:

$$S_{11}'=Q(u_1,v_1)=\lambda_1\ .\ D=n_1\sqrt{S'}\ .$$

In other words, we have to look for numbers $Q(u_1,v_1)$ [defined by equation (20)] which are divisible by $\sqrt{S'}$. Such numbers exist in every case. Since the elements S_{ij} are integer, there exists another vector $\mathbf{r}(u_2,v_2)$ which is perpendicular (but not necessarily equal) to the vector $\mathbf{r}(u_1,v_1)$. If $Q(u_2,v_2)=\lambda_2\ .\ D=n_2\ .\ \sqrt{S'}$ we have according to equation (23):

$$Q(u_1,v_1)\ .\ Q(u_2,v_2)=D^2S'=n_1\ .\ n_2\ .\ S'=\lambda_1\lambda_2\ .\ D^2.$$

Since S' is a square the normalized metric tensor of the rectangle formed by the vectors $\mathbf{r}_1(u_1,v_1)$ and $\mathbf{r}_2(u_2,v_2)$ is a square, $Q(u_1,v_2)$ and $Q(u_2,v_2)$ have the ratio of squares, so that it is possible to get a square from this rectangle by multiplying one of its edges or both.

We wish to emphasize that any square mesh possesses non-trivial square supermeshes. Its indices are given by the so-called tetragonal numbers, *i.e.* all integers which are the sums of two squares. The vectors $[u,v]$ and $[v,\bar{u}]$ of a square net are the edges of a non-trivial square supermesh. From Theorem 3 it follows that a hexagonal mesh does not possess a square supermesh because the determinant of its normalized metric tensor is equal to 3. The next theorem states the conditions for the existence of a hexagonal supermesh of a given net.

Theorem 4

A mesh possesses a hexagonal supermesh if and only if the elements s_{ij} of its metric tensor have the ratio of integers S_{ij} and if the determinant of the normalized metric tensor $\mathbf{S}'=\{S_{ij}\}$ is the threefold of a square number.

Proof: A hexagonal mesh can be regarded as the primitive mesh of a centred rectangular net the squared edges of which have the ratio 1:3. This rectangular net has also a hexagonal twofold supermesh formed by the vectors [1,1] and $[1,\bar{1}]$. Bearing this in mind the proof can be accomplished in analogy with the proof of the former theorem.

It is emphasized that any hexagonal mesh [characterized by the normalized metric tensor $\binom{2\bar{1}}{\bar{1}2}$] has non-trivial hexagonal supermeshes. Any vector $[u,v]$ of the hexagonal net forms, together with the vector $[v-u, -u]$ a hexagonal supermesh with the index $D=u^2-uv+v^2$.

In Tables 2 and 3 the square supermeshes of the reduced non-rectangular meshes with normalized discriminants $S'\leq 100$ and the hexagonal supermeshes of all non-rectangular and non-hexagonal meshes with normalized discriminants $S'\leq 300$ are given. A mesh is called reduced if and only if the elements s_{ij} of its metric tensor satisfy the condition $2|s_{12}|\leq s_{11}\leq s_{22}$ (Niggli, 1928).

These Tables suggest the following rules: (1) The index D of the smallest square supermesh of a mesh with the normalized discriminant S' is equal to $D=$

$\sqrt{S'}$; (2) The index D of the smallest hexagonal supermesh of a mesh with the normalized discriminant S' is equal to $D=\sqrt{S'/3}$, if the elements S_{11} and S_{22} of its normalized metric tensor S' are even; otherwise it is equal to $D=2\sqrt{S'/3}$. Because the conditions of Theorems 3 and 4 are mutually exclusive they imply the following corollary:

Corollary: No mesh can simultaneously possess square and hexagonal supermeshes.

As we shall see in the following section this corollary does not hold for a three-dimensional cell, *i.e.* a cell can possess hexagonal and tetragonal supercells.

Table 2. *Square supermeshes of all reduced non-rectangular meshes with a normalized discriminant* $S' \le 100$

S'	S_{11}	S_{22}	S_{12}	u_1	v_1	u_2	v_2	D
9	2	5	1	1	1	$\bar{2}$	1	3
16	4	5	2	1	$\bar{2}$	2	0	4
25	2	13	1	2	1	$\bar{3}$	1	5
36	5	8	2	2	1	$\bar{2}$	2	6
49	2	25	1	3	1	$\bar{4}$	1	7
49	5	10	1	3	$\bar{1}$	1	2	7
64	5	13	1	3	1	$\bar{2}$	2	8
64	4	17	2	1	$\bar{2}$	4	0	8
81	2	41	1	4	1	$\bar{5}$	1	9
81	5	17	2	4	$\bar{1}$	1	2	9
81	9	10	3	$\bar{1}$	3	3	0	9
100	8	13	2	3	$\bar{2}$	2	2	10

Table 3. *Hexagonal supermeshes of all reduced non-rectangular meshes with a normalized discriminant* $S' \le 300$

S'	S_{11}	S_{22}	S_{12}	u_1	v_1	u_2	v_2	D
27	2	14	1	2	$\bar{1}$	$\bar{3}$	0	3
27	4	7	1	$\bar{3}$	0	1	2	6
48	7	7	1	3	$\bar{1}$	$\bar{1}$	3	8
48	4	13	2	1	2	$\bar{3}$	2	8
75	2	38	1	$\bar{3}$	1	5	0	5
75	4	19	1	$\bar{3}$	2	5	0	10
75	7	12	3	$\bar{2}$	3	4	$\bar{1}$	10
75	6	14	3	$\bar{1}$	2	3	$\bar{1}$	5
108	7	16	2	4	$\bar{1}$	0	3	12
108	9	13	3	1	3	3	$\bar{3}$	12
147	4	37	1	$\bar{7}$	0	3	2	14
147	2	74	1	$\bar{4}$	1	7	0	7
147	6	26	3	$\bar{1}$	2	4	$\bar{1}$	7
147	12	13	3	3	2	1	$\bar{4}$	14
192	4	49	2	3	2	5	$\bar{2}$	16
192	7	28	2	$\bar{2}$	3	6	$\bar{1}$	16
192	13	16	4	$\bar{4}$	3	4	1	16
192	12	19	6	$\bar{5}$	2	3	2	16
243	2	122	1	$\bar{5}$	1	9	0	9
243	4	61	1	$\bar{5}$	2	9	0	18
243	13	19	2	5	$\bar{1}$	$\bar{2}$	4	18
243	7	36	3	$\bar{6}$	2	6	1	18
243	9	28	3	2	3	4	$\bar{3}$	18
243	14	18	3	$\bar{3}$	2	3	1	9
300	7	43	1	7	1	$\bar{1}$	$\bar{3}$	20
300	16	19	2	$\bar{3}$	4	5	0	20
300	13	25	5	$\bar{5}$	3	5	1	20
300	16	21	6	$\bar{5}$	0	1	4	20

3. Orthogonal supercells of a cell

A cell is called orthogonal if one of its edges is orthogonal to the two others, *i.e.* if it has at least monoclinic symmetry. A lattice possesses an orthogonal supercell if and only if one of its vectors $\mathbf{r}(\mathbf{u})=u\mathbf{a}_1+v\mathbf{a}_2+w\mathbf{a}_3$ is perpendicular to a lattice plane defined by the vector $\mathbf{r}^*(\mathbf{h})=h\mathbf{a}_1^*+k\mathbf{a}_2^*+l\mathbf{a}_3^*$ of its reciprocal lattice. In this case equation (17) (which holds also for a space lattice as is easily proven) is satisfied. This condition can be formulated in the following way: A lattice possesses an orthogonal supercell if and only if there exists a lattice vector $\mathbf{r}(\mathbf{u})$ such that the vector $\mathbf{Su}$ is proportional to an integer vector $\mathbf{h}$. This vector gives the indices of the lattice plane perpendicular to $\mathbf{r}(\mathbf{u})$. This perpendicularity condition is equivalent to the conditions given in *International Tables for X-ray Crystallography* (1959). If all elements $s_{ij}(i,j=1,2,3)$ of the metric tensor S have the ratio of reasonably small integers S_{ij}, condition (17) is satisfied for every lattice vector $\mathbf{r}(\mathbf{u})$. But even if there does not exist such an integer ratio among the elements s_{ij} there may exist an orthogonal supercell. Such a supercell can be found in the following way: first two vectors $\mathbf{r}_1(\mathbf{u}_1)$ and $\mathbf{r}_2(\mathbf{u}_2)$ are to be found which have the same length. Then the vectors $\mathbf{r}_1+\mathbf{r}_2$ and $\mathbf{r}_1-\mathbf{r}_2$ are perpendicular to each other. An orthogonal supercell with one of these vectors as the unique axis exists if $\mathbf{S}(\mathbf{u}_1+\mathbf{u}_2)$ or $\mathbf{S}(\mathbf{u}_1-\mathbf{u}_2)$ is proportional to an integer vector $\mathbf{h}=(h,k,l)$. The primitive reduced mesh of the (h,k,l) plane then forms together with the vector $\mathbf{u}_1+\mathbf{u}_2$ (or $\mathbf{u}_1-\mathbf{u}_2$) an orthogonal supercell. This procedure will be illustrated by the following numerical example. Let the metric tensor of a triclinic cell be

$$\mathbf{S}=\begin{pmatrix} 3\cdot123 & 0\cdot411 & 0\cdot160 \\ 0\cdot411 & 3\cdot480 & 0\cdot517 \\ 0\cdot160 & 0\cdot517 & 4\cdot051 \end{pmatrix}.$$

The vectors $\mathbf{r}_1=[20\bar{1}]$ and $\mathbf{r}_2=[02\bar{1}]$ have the same length, namely $\sqrt{15\cdot903}$. Consequently the vectors $\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)=[11\bar{1}]$ and $\frac{1}{2}(\mathbf{r}_1-\mathbf{r}_2)=[1\bar{1}0]$ are perpendicular to each other. The vector $\frac{1}{2}\mathbf{S}(\mathbf{u}_1+\mathbf{u}_2)$ becomes (3·374, 3·374, −3·374), which is proportional to the vector $(h,k,l)=(11\bar{1})$. This means that the $(11\bar{1})$ plane is normal to the lattice vector $[11\bar{1}]$. This net plane is formed by the vectors $[1\bar{1}0]$ and $[101]$, the former of which is equal to $\frac{1}{2}(\mathbf{r}_1-\mathbf{r}_2)$. The cell formed by the vectors $\mathbf{a}_1'=[1\bar{1}0]$, $\mathbf{a}_2'=[11\bar{1}]$ and $\mathbf{a}_3'=[101]$ is a threefold monoclinic supercell of the original cell with the metric tensor,

$$\mathbf{S}'=\begin{pmatrix} 5\cdot781 & 0\cdot0 & 2\cdot355 \\ 0\cdot0 & 10\cdot122 & 0\cdot0 \\ 2\cdot355 & 0\cdot0 & 7\cdot494 \end{pmatrix}.$$

The existence of an orthogonal supercell is obviously a necessary condition for twinning. According to *Inter-*

national Tables a triclinic lattice can twin only if the elements s_{ij} of its metric tensor, *i.e.* if

$$a^2:b^2:c^2:bc\cos\alpha:ac\cos\beta:ab\cos\gamma\,,$$

have the ratio of sufficiently small integers. As our example shows this condition is not necessary.

By the methods of § 2 it can be shown that the (010) plane of this monoclinic supercell possesses a fivefold rectangular supermesh because $3s'_{11}-2s'_{33}-s'_{13}=0$ (see Theorem 1). According to equations (11) and (12) the vectors $[u_1,0,v_1]=[1,0,\bar{1}]$ and $[u_2,0,v_2]=[3,0,2]$ of the monoclinic supercell, corresponding to the vectors $[0\bar{1}\bar{1}]$ and $[5\bar{3}2]$ of the original cell, are perpendicular to each other. Together with the vector [010] of the monoclinic cell (or $[11\bar{1}]$ of the original cell) they form a 15-fold orthorhombic supercell of the original cell.

The most interesting supercells are cubic, hexagonal and tetragonal. The necessary and sufficient conditions for the existence of such supercells will now be derived.

3.1 *Cubic supercells*

A cubic supercell exists only if the elements s_{ij} of the metric tensor of the original cell have the ratio of integers S_{ij}. These integers S_{ij} which are supposed to possess no common divisor $\neq 1$ are the elements of the 'normalized' metric tensor $\mathbf{S}'$. The determinant of the metric tensor $\mathbf{S}$ is equal to the square of the volume of the unit cell. Introducing a *cell matrix*

$$\mathbf{C}=\begin{pmatrix}\mathbf{a}_1\\\mathbf{a}_2\\\mathbf{a}_3\end{pmatrix} \qquad (26)$$

in analogy to the mesh matrix $\mathbf{M}$ of equation (5) and an integer transformation matrix $\mathbf{T}_{21}$ for the transformation of the original cell $\mathbf{C}_1$ into a supercell $\mathbf{C}_2$, defined by

$$\mathbf{C}_2=\mathbf{T}_{21}\mathbf{C}_1\,, \qquad (27)$$

we obtain for the matric tensor $\mathbf{S}_2$ of the supercell, in analogy with equations (6) and (22):

$$\mathbf{S}_2=\mathbf{C}_2\tilde{\mathbf{C}}_2=\mathbf{T}_{21}\mathbf{C}_1\tilde{\mathbf{C}}_1\tilde{\mathbf{T}}_{21}=\mathbf{T}_{21}\mathbf{S}_1\tilde{\mathbf{T}}_{21}\,.$$

From this equation follows at once that

$$|\mathbf{S}_2|=|\mathbf{T}_{21}|^2\,.\,|\mathbf{S}_1|\,. \qquad (28)$$

We replace the metric tensor $\mathbf{S}_1$ by the normalized tensor $\mathbf{S}'_1$. If the supercell $\mathbf{S}_2$ is to be cubic the tensor $\mathbf{S}'_2=\mathbf{T}_{21}\mathbf{S}'_1\tilde{\mathbf{T}}_{21}$ must be an integer multiple of the unit matrix. We get, therefore, from (28)

$$|\mathbf{S}'_2|=n^3=D^2\,.\,|\mathbf{S}'_1|,\quad\text{with}\quad D=|\mathbf{T}_{21}|\ \text{integer}\,. \qquad (29)$$

Equation (29) provides a necessary condition for the possible values of D and of n. The smallest possible value of D is $|\mathbf{S}'_1|/d^3$, where d^3 is the greatest cubic divisor of $|\mathbf{S}'_1|$. n is then equal to $|\mathbf{S}'_1|/d^2$. If condition (29) is satisfied for D and n it is also satisfied for the values $D'=m^3D$ and $n'=m^2n$, where m is an arbitrary integer. n is obviously the square of the edge of the possible cubic supercell of the 'normalized' original lattice defined by $\mathbf{S}'$. Now we have to look for vectors $\mathbf{r}(\mathbf{u})$ of this lattice with $|\mathbf{r}(\mathbf{u})|^2=n$. The integer vectors $\mathbf{S}'_1\mathbf{u}=\lambda\mathbf{h}$ (λ integer) define the Miller indices of the planes perpendicular to these vectors. The scalar product $\mathbf{h}\,.\,\mathbf{u}$ must be a divisor of D if there is to exist a D-fold cubic supercell. Furthermore, the net plane $\mathbf{h}$ must contain another vector $\mathbf{r}'(\mathbf{u}')$ with $\mathbf{r}'^2=n$. If this is the case there exists a third vector $\mathbf{r}''(\mathbf{u}'')$ in the same net-plane which together with the vectors $\mathbf{r}$ and $\mathbf{r}'$ forms a cubic supercell. The indices of $\mathbf{r}''$ are readily found by forming the cross product of $\mathbf{h}$ with $\mathbf{h}'=\mathbf{S}'\mathbf{u}'$, because the planes $\mathbf{h}$ and $\mathbf{h}'$ intersect in the third vector.

As an example let us calculate the cubic supercell of the lattice with the normalized metric tensor

$$\mathbf{S}'=\begin{pmatrix}6&2&3\\2&9&1\\3&1&14\end{pmatrix}.$$

Since the determinant $S'=625=5^4$, the smallest possible values of D and n are $D=5$ and $n=25$. The vector $\mathbf{r}=[011]$ satisfies the condition $\mathbf{r}^2=25$. This vector is perpendicular to the plane $\mathbf{S}'\mathbf{u}=(123)$. In the (123) plane we find the vector $\mathbf{r}'=[11\bar{1}]$ with $\mathbf{r}'^2=25$. This vector is perpendicular to the $(12\bar{2})$ plane. The (123) plane and the $(12\bar{2})$ plane intersect in the vector $[2\bar{1}0]$, which is the third edge of the cubic supercell.

A cubic cell possesses non-trivial cubic supercells, the smallest of which is the 27-fold cell with the edges [221], $[1\bar{2}2]$ and $[2\bar{1}\bar{2}]$.

3.2 *Hexagonal supercells*

A necessary condition for the existence of a hexagonal supercell of a lattice is the existence of three coplanar lattice vectors $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{r}_3$ of equal length such that $\mathbf{r}_1+\mathbf{r}_2=\mathbf{r}_3$. If such vectors exist each of them must furthermore be perpendicular to a net-plane of the given lattice, *i.e.* the vectors $\mathbf{Su}_1$, $\mathbf{Su}_2$, $\mathbf{Su}_3$ must be proportional to integer vectors $\mathbf{h}_1$, $\mathbf{h}_2$ and $\mathbf{h}_3$ respectively. The hexagonal axis is then given by the cross product of any two vectors $\mathbf{h}_i$.

Let the elements s_{ij} of the metric tensor $\mathbf{S}$ have the ratio of integers, and let $\mathbf{S}^\times$ be the adjoint matrix of the normalized metric tensor $\mathbf{S}'$. In this case a hexagonal supercell exists if and only if there exists a number $F=\mathbf{hS}^\times\mathbf{h}$ (with integer column vector $\mathbf{h}$) which is a threefold squared integer. In this case the netplane defined by $\mathbf{h}$ possesses a hexagonal supermesh according to Theorem 4. (The values of F are the squares of the mesh areas of the net-planes of the normalized lattice and therefore identical with their discriminants). The coordinates of its edges in terms of the reduced basic vectors of this net-plane can be taken from Table 3, if $F\leq 300$ and if its mesh is not rectangular. The hexagonal axis $\mathbf{u}$ is determined as in the general case described above, or by the equation $\mathbf{u}=\mathbf{S}^\times\,.\,\mathbf{h}$, which can be derived from the three-dimensional analogue of equation (15).

As an example we take a monoclinic lattice with the normalized metric tensor

$$\mathbf{S}'=\begin{pmatrix}2&1&1\\1&3&1\\1&1&4\end{pmatrix}.$$

Its adjoint matrix is

$$\mathbf{S}^{\times}=\begin{pmatrix}11&\bar{3}&\bar{2}\\\bar{3}&7&\bar{1}\\\bar{2}&\bar{1}&5\end{pmatrix}.$$

Its (101) plane has the discriminant $F=12$ and possesses, therefore, a hexagonal supermesh. The mesh of the (101) plane is formed by the vectors [010] and [10$\bar{1}$], its metric tensor becomes $\binom{3\,0}{0\,4}$. The hexagonal supermesh is formed by the vectors [21] and [$\bar{2}$1] in terms of the net, that is by the lattice vectors [12$\bar{1}$] and [1$\bar{2}\bar{1}$]. The (101) plane is perpendicular to the lattice vector [9$\bar{4}$3]. We obtain, therefore, a 48-fold hexagonal supercell by the transformation

$$\mathbf{T}=\begin{pmatrix}1&2&\bar{1}\\1&\bar{2}&\bar{1}\\9&\bar{4}&3\end{pmatrix}.$$

There exists another 48-fold hexagonal supercell based on the (110) plane which is obtained by the transformation

$$\mathbf{T}=\begin{pmatrix}2&\bar{2}&1\\\bar{2}&2&1\\8&4&\bar{3}\end{pmatrix}.$$

3.3 *Tetragonal supercells*

A tetragonal supercell of a lattice exists if and only if there are two lattice vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ of equal lengths such that $|\mathbf{r}_1+\mathbf{r}_2|^2=2\mathbf{r}_1^2=2\mathbf{r}_2^2$ and if each of these vectors is perpendicular to a lattice plane, $\mathbf{h}_1$ and $\mathbf{h}_2$ respectively. The intersection vector of these planes is the tetragonal axis.

The case of an integer-normalized metric tensor $\mathbf{S}'$ is treated in complete analogy with the hexagonal case. In this case $F=\mathbf{h}\mathbf{S}^{\times}\mathbf{h}$ must, of course, be a squared integer. A hexagonal lattice may possess tetragonal supercells, and *vice versa*. The hexagonal cell with the normalized metric tensor

$$\mathbf{S}=\begin{pmatrix}2&\bar{1}&0\\\bar{1}&2&0\\0&0&2\end{pmatrix},$$

for instance, possesses a twofold tetragonal supercell with the metric tensor

$$\begin{pmatrix}2&0&0\\0&2&0\\0&0&6\end{pmatrix},$$

which is obtained by the transformation

$$\mathbf{T}=\begin{pmatrix}0&1&0\\0&0&1\\2&1&0\end{pmatrix}.$$

The normalized metric tensor of that hexagonal cell is typical for the WC structure type.

4. Applications

As already mentioned, orthogonal supercells are a necessary condition for any type of twinning. Twinned lattices are a special case of coincidence-site lattices which play a certain role in the theory of large-angle grain boundaries (Acton & Bevis, 1971). A lattice possesses a coincidence-site lattice of the non-twinning type if and only if it possesses an orthorhombic supercell with at least one axial ratio R such that R^2 is rational (Fortes, 1972). In a previous paper (Bucksch 1972) a method was presented by means of which the greatest common subcell and the smallest common supercell of two lattices can be calculated. In practical cases these common subcells and supercells of polymorphs or related structures frequently possess higher metric symmetries than the original cells, often of approximately cubic or hexagonal symmetry. It was just this observation which stimulated the present paper. As Niggli (1949) pointed out, 'there exists a far-reaching morphological relationship among the structure types as could be established among different phenomenological types with regard to symmetry and metrics'. This relationship can often be deduced from the existence of subcells of higher symmetry. These subcells can be found by applying the methods of this paper to the reciprocal cells and transforming them back to the direct cells. Owing to some distortions (up to about 10% in the lengths of the edges and 5° in the angles) accompanying the transition to lower symmetries the elements of the metric tensor can be varied a little before applying the criteria of §§ 2 and 3. If an approximately cubic supercell or subcell is to be found the parameters D and n of condition (29) are to be made as small as possible by a proper variation of the metric tensor within the permitted limits. In the orthorhombic phase of $BaNb_2O_6$, for instance, $a^2:b^2:c^2$ is approximately 24:17:10. By a small variation we get the ratio 24:18:9=8:6:3, from which we get the ratio $a^{*2}:b^{*2}:c^{*2}=3:4:8$ for the reciprocal cell, so that $\mathbf{S}_1'$ becomes 96, $D=12$ and $n=24$ according to (29). The vectors (021), (21$\bar{1}$) and (2$\bar{1}$1) form a cubic supercell of the reciprocal cell, corresponding to an approximately cubic subcell of the direct cell with the edges $\frac{1}{3}$[011], $\frac{1}{12}$[32$\bar{4}$] and $\frac{1}{12}$[3$\bar{2}$4]. Filling this subcell with a NbO_6 octahedron in analogy with the perovskite structure, putting it in an appropriate region of the orthorhombic $BaNb_2O_6$ cell and applying the symmetry operations of the orthorhombic cell to these atoms we obtain a first approximation to the $BaNb_2O_6$ structure. The reflexion by the orthorhombic (100) plane corresponds to a reflexion by the cubic $(01\bar{1})$ plane. More details of this particular application will be given in another paper.

Every net-plane of a cubic, tetragonal or hexagonal lattice is either orthogonal or possesses an n-fold orthogonal supermesh, where n is a primitive tetragonal (hexagonal or double hexagonal) number in the case of a tetragonal (or hexagonal) lattice. Primitive tetragonal (hexagonal) numbers are represented by the quadratic forms u^2+v^2 (u^2+uv+v^2), where u and v are relatively prime. The orthogonal supercell of a tetragonal (hexagonal) (hkl) plane is formed by the lattice vectors $[k,\bar{h},0]$ and $[hl,kl,-(h^2+k^2)]$ (or $[l(k+2h), l(2k+h),-2(h^2+hk+k^2)]$ in the hexagonal case). This supermesh of the (hkl) plane is (h^2+k^2)-fold in the tetragonal case and $2(h^2+hk+h^2)$-fold in the hexagonal case. The indices of each of these vectors should be divided by their common divisor. If l is even, the orthogonal supermesh of a hexagonal net-plane thus becomes (h^2+hk+h^2)-fold. In a hexagonal (hhl) plane this supermesh becomes two fold, if l is odd, otherwise the net-plane is orthogonal. Any divisor of a tetragonal (or hexagonal) number is again a tetragonal (or hexagonal) number. Consequently the statement given above remains true. In the case of a rational $c^2:a^2$ ratio there may exist orthogonal supermeshes smaller than those given above.

With the aid of these facts we can decide by the application of Theorem 1 whether a given mesh (as for instance of a zonal plane obtained by selected electron diffraction or by a general procedure of indexing powder patterns) can belong to a tetragonal or hexagonal lattice or not, and we can calculate the small number of tetragonal or hexagonal lattices which contain this mesh. Another mesh of the same lattice will in general permit a unique choice among these possible lattices, which is then to be verified by a third mesh.

All net-planes of a lattice which possesses a tetragonal or hexagonal supercell have supermeshes of the corresponding sublattices and consequently also orthogonal supermeshes. This fact provides an additional criterion for the existence of cubic, tetragonal and hexagonal supercells.

Finally the algebraic method of converting reduced cells to conventional supercells (Bucksch, 1971) can be simplified by the methods presented in this paper, especially by application of equations (17) to (19).

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