the correspondence $m_y \leftrightarrow m_\alpha$, namely $\alpha \leftrightarrow y$. Hence, C_y appears in the first line (under m_α), and the magnetic group according to which C_y (C_α) transforms is (Table 4) *Pnma* ($m_\alpha m_\beta m_\gamma$).

References

BERTAUT, E. F. (1968). *Acta Cryst.* A**24**, 217.

GUREWITZ, E., MAKOVSKY, J. & SHAKED, H. (1972). To be published.

GUREWITZ, E. & SHAKED, H. (1971). *Limiting Conditions on Possible Reflections from Magnetic Configurations in* D^i_{2h}, $i=1,2,\ldots 16$, NRCN 316.

International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.

SHIRANE, G. (1959), *Acta Cryst.* **12**, 282.

Acta Cryst. (1972). A**28**, 284

Properties of Crystal Lattices: The Derivative Lattices and their Determination

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Derivative lattices are classified as super, sub and composite, on the basis of the properties of the transformation matrices relating them to the lattice from which they are derived. A method for obtaining the transformation matrices generating these lattices is given. The method has been applied to the derivation of the unique super and sublattices in a few important cases.

The super and sublattices associated with the lattice of a crystal are not infrequently related to important properties of the crystal. For example, in the case of twinning by reticular merohedry, twinning takes place only if a superlattice possesses symmetry (or pseudosymmetry) higher than that of the crystal lattice (Friedel, 1964; Donnay, Donnay & Kullerud, 1958). The concepts of super and sublattices are also essential in the study of some derivative structures (Buerger, 1946, 1954). In an order–disorder transformation, for example, the ordered phase is characterized by a cell larger than that of the disordered phase and, similarly, the cell on which a magnetic structure is based is often larger than that of the corresponding chemical structure. So far, no attempt has been made to determine systematically the number and the geometrical properties of super and sublattices associated with a given lattice, and the treatment of this subject has been generally restricted to specific cases of interest. In this paper, we define derivative lattices and then outline a method for their derivation.

Let us consider any given lattice and let us describe it in terms of any arbitrary primitive triplet of noncoplanar translations $\mathbf{a}_i$ (a triplet is called *primitive* when it defines a primitive cell: *International Tables for X-ray Crystallography*, 1969, p. 8). Let us now perform the axial transformation

$$\mathbf{b}_i=\textstyle\sum_j S_{ij}\mathbf{a}_j \; (i,j=1,2,3) \qquad (1)$$

and let us assume that the determinant $|\mathrm{S}|$ of the transformation matrix S is different from zero. The three noncoplanar translations $\mathbf{b}_i$ can be regarded as the edges of a primitive cell defining a new lattice related to the one based on the translations $\mathbf{a}_i$ by transformation (1). We may call *original lattice* the lattice based on the triplet of translations $\mathbf{a}_i$ and *derivative lattice* the lattice defined by the triplet of translations $\mathbf{b}_i$, provided that this triplet is considered primitive. Original and derivative lattices are in general different, *i.e.* they have different reduced cells (Niggli, 1928; *International Tables for X-ray Crystallography*, 1969, p. 530). However, if the elements S_{ij} are integers, and if the determinant $|\mathrm{S}|$ is equal to unity, the two lattices are identical.

The derivative lattices of interest in crystallography are those that are obtained when the elements S_{ij} in transformation (1) are simple rational numbers. These lattices can be defined in terms of the properties of the transformation matrix S as follows.

Definition 1. A derivative lattice is a *superlattice*,* if the elements S_{ij} of matrix S are integers, and if the determinant $|\mathrm{S}|$ is greater than one. Thus, all the nodes of the superlattice are nodes of the original lattice, but not all nodes of the original lattice are nodes of the superlattice.

Definition 2. Let **T** be the inverse of matrix **S**, *i.e.* $\mathbf{T}=\mathbf{S}^{-1}$. A derivative lattice is a *sublattice*, if the elements T_{ij} of matrix **T** are integers, and if the determinant $|\mathbf{T}|$ is greater than one. Thus all the nodes of

* In some publications, especially in the mathematical literature (*e.g.* Cassels, 1959), a 'superlattice' as defined in this paper is called a sublattice because it is generated by a subgroup of the translations on which the original lattice is based.

the original lattice are also nodes of the sublattice, but not all the nodes of the sublattice are nodes of the original lattice.

Definition 3. A derivative lattice is a *composite lattice*, if one or more of the elements S_{ij} of matrix **S**, and one or more of the elements T_{ij} of matrix **T** are fractional. A composite lattice, therefore, is neither a superlattice, nor a sublattice, although it partakes of the two.

Matrix **S** in expression (1) transforms a given cell of the original lattice into a given cell of the derivative lattice. The same derivative lattice can be described in terms of an infinite number of primitive cells, and it can be obtained from an infinite number of primitive cells of the original lattice. In other words the lattice generated by a matrix **S** can also be generated by any one of the matrices **S**′ given by the equation:

$$\mathbf{S}'=\mathbf{HSK}\,, \tag{2}$$

where the elements H_{ij} and K_{ij} of matrices **H** and **K** are integers, and the determinants $|\mathbf{H}|$ and $|\mathbf{K}|$ are equal to one. [In equation (2), matrix **K** relates, in the original lattice, the two cells transformed by matrices **S** and **S**′, and matrix **H** relates, in the derivative lattice, the two cells produced by these transformations.] Matrices **S** and **S**′ not related by equation (2) generate different derivative lattices, either of different type (*e.g.* a superlattice and a sublattice), or of the same type with $|\mathbf{S}|\neq|\mathbf{S}'|$ or with $|\mathbf{S}|=|\mathbf{S}'|$. These matrices are easily recognizable because matrix $\mathbf{S}'(\mathbf{SK})^{-1}$ has nonintegral elements and/or a determinant different from one.

The determination of super, sub and composite lattices requires finding the unique matrices **S** that generate these lattices for any given value of the determinant of the transformation.

We will consider first the derivation of superlattices. The transformation of coordinates corresponding to transformation (1) is (*International Tables for X-ray Crystallography*, 1969, p. 15):

$$\boldsymbol{\beta}=\tilde{\mathbf{T}}\boldsymbol{\alpha} \tag{3}$$

where $\tilde{\mathbf{T}}$ is the transpose of **T**, and $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$ are the column vectors formed by the coordinates β_i and α_i of a point referred to the reference systems $\mathbf{b}_i$ and $\mathbf{a}_i$ respectively. The nodes of the superlattice have integral coordinates. (Points with fractional β_i are not nodes of the superlattice, although they may be nodes of the original lattice. This is a consequence of assuming that the translations $\mathbf{b}_i$ define a primitive cell.) Indicating with $\bar{\mathbf{S}}$ the adjoint of **S** ($\bar{\mathbf{S}}=|\mathbf{S}|\mathbf{T}$), we have from (3):

$$|\mathbf{S}|\boldsymbol{\beta}=\tilde{\bar{\mathbf{S}}}\boldsymbol{\alpha}\,. \tag{4}$$

Equation (4) shows that the coordinates α_i of points that are nodcs of a superlattice must be such that $\sum_j\bar{\mathbf{S}}_{ji}\alpha_j$ are integral multiples of the determinant $|\mathbf{S}|$ of the transformation that generates the superlattice. Conditions (4), therefore, limit the possible values which the α_i can assume in much the same way as the conditions on h,k,l limit the possible reflexions in the determination of lattice types from diffraction patterns. However, the conditions defining all the unique superlattices consistent with a given value of $|\mathbf{S}|$ cannot easily be found by using expression (4). This can be understood by remembering that a derivative lattice can be generated by any of the matrices given by equation (2). Therefore, the values that the elements $\bar{S}_{ji}$ can assume in (4) are infinite in number. To circumvent this problem, we have to find a uniquely defined matrix to be taken as a representative of the entire class of matrices related by equation (2).

One way to accomplish this result is by introducing a matrix **L**, defined by the expression

$$\mathbf{L}=\bar{\mathbf{S}}-|\mathbf{S}|\mathbf{N}\,, \tag{5}$$

in which **N** is a matrix with integral elements chosen so that the elements L_{ij} obey the following condition:

$$\begin{aligned}\frac{2-|\mathbf{S}|}{2}&\le L_{ij}\le\frac{|\mathbf{S}|}{2}\text{ for }|\mathbf{S}|\text{ even,}\\[2ex]\frac{1-|\mathbf{S}|}{2}&\le L_{ij}\le\frac{|\mathbf{S}|-1}{2}\text{ for }|\mathbf{S}|\text{ odd.}\end{aligned} \tag{6}$$

Equation (4) can be written:

$$|\mathbf{S}|\beta_i=\textstyle\sum_j\bar{\mathbf{S}}_{ji}\alpha_j=\sum_jL_{ji}\alpha_j+|\mathbf{S}|\sum_jN_{ji}\alpha_j, \tag{7}$$

and from this we obtain:

$$\textstyle\sum_jL_{ji}\alpha_j=|\mathbf{S}|(\beta_i-\sum_jN_{ji}\alpha_j)=n_i|\mathbf{S}|\,, \tag{8}$$

where the coefficients n_i are integers. Conditions (8), like conditions (3), define a superlattice by eliminating some of the nodes of the original lattice. More precisely, points whose coordinates α_i satisfy (8) are nodes of a superlattice as well as nodes of the original lattice, while points with integral coordinates α_i that do not satisfy (8) are nodes of the original lattice but not of the superlattice. It can be shown that if in (2) we impose the condition $\mathbf{K}=\mathbf{I}$, where **I** is the identity matrix, the matrices generating the same superlattice, and only these matrices, produce the same set of conditions (8). Therefore, the problem of deriving the unique superlattices for any given value of $|\mathbf{S}|$ consists in finding all the unique matrices $\tilde{\mathbf{L}}$ consistent with that value of $|\mathbf{S}|$, provided that the transformations generating the superlattices are applied to the same cell of the original lattice ($\mathbf{K}=\mathbf{I}$).

The main limitation on the number of matrices $\tilde{\mathbf{L}}$ consistent with a given $|\mathbf{S}|$ is imposed by the fact that the possible values of the elements L_{ij} are limited by conditions (6). For example, for $|\mathbf{S}|=2$, the elements L_{ij} can be zero or one; for $|\mathbf{S}|=3$, they can be -1, 0, or 1, *etc.* The possible values of the elements L_{ij} for a given value of $|\mathbf{S}|$ are first grouped in sets of three to form the rows (L_{1i},L_{2i},L_{3i}) of matrix $\tilde{\mathbf{L}}$. Note that the order in which this grouping is done is relevant. For example, the rows (0,0,1) and (0,1,0) are different, as they correspond to the conditions $\alpha_3=n|\mathbf{S}|$ and $\alpha_2=m|\mathbf{S}|$ respectively. On the other hand, not all the possible rows are unique. For example, the rows $(-L_{1i}, -L_{2i}, -L_{3i})$ and (L_{1i}, L_{2i}, L_{3i}) are equivalent, *i.e.* they imply the same condition $L_{1i}\alpha_1+L_{2i}\alpha_2+L_{3i}\alpha_3=n|\mathbf{S}|$ and therefore one of them has to be rejected to avoid duplication. Similarly, for $|\mathbf{S}|$ even, the rows $[-L_{1i}, -L_{2i}, (|\mathbf{S}|/2)]$ and $[L_{1i}, L_{2i}, (|\mathbf{S}|/2)]$ are equivalent, and other types of equivalence can easily be discovered case by case. The order in which the rows are combined to form the matrices $\tilde{\mathbf{L}}$ is irrelevant; matrices 001/000/000 and 000/001/000 both imply $\alpha_3=n|\mathbf{S}|$, so that only one matrix needs to be considered. Furthermore, not all the matrices $\tilde{\mathbf{L}}$ are unique. For example, matrix 001/001/000 implies $\alpha_3=n|\mathbf{S}|$ as does matrix 001/000/000; one of them can therefore be eliminated. Finally, some of the matrices $\tilde{\mathbf{L}}$ are inconsistent with the value of $|\mathbf{S}|$ under consideration and have to be ignored. Matrix 001/010/000, for example, implies $\alpha_3=n|\mathbf{S}|$ and $\alpha_2=m|\mathbf{S}|$ simultaneously and, as a consequence, defines a superlattice of determinant $(|\mathbf{S}|)^2$. Such a matrix must be rejected if the superlattices being determined are characterized by determinant $|\mathbf{S}|$. After this systematic process of elimination has been accomplished, the remaining matrices $\mathbf{L}$ define, through conditions (8), all the unique superlattices consistent with a given value of $|\mathbf{S}|$. The matrices $\mathbf{S}$, corresponding to the matrices $\mathbf{L}$, can be obtained from the equation

$$\bar{\mathbf{S}}=\mathbf{L}+|\mathbf{S}|\mathbf{N} \tag{9}$$

and

$$\mathbf{S}=|\mathbf{S}|(\bar{\mathbf{S}})^{-1}. \tag{10}$$

The elements N_{ij} of matrix $\mathbf{N}$ in (9) must be chosen so that $|\bar{\mathbf{S}}|=(|\mathbf{S}|)^2$, but they are otherwise arbitrary. In fact, it can be shown that a superlattice is completely defined by matrix $\mathbf{L}$ and that matrix $\mathbf{N}$ merely defines the cell describing the superlattice. The unique matrices $\mathbf{S}$, and the corresponding conditions (8) on the α_i, are presented in Table 1 for $|\mathbf{S}|=2,3,4$.

Matrices that satisfy definition (2) for sublattices can be obtained by calculating the inverses of the matrices given in Table 1. In this way, however, one does not obtain all the unique sublattices associated with the original lattice. For example, the transformations (200/010/001) and (200/110/001) define two different superlattices when applied to the same original cell, but the inverse matrices ($\frac{1}{2}$00/010/001) and ($\frac{1}{2}$00/$-\frac{1}{2}$10/001), define two different cells of the same sublattice.

The matrices generating the unique sublattices can be derived with the help of the reciprocal lattice. The original cell, based on the primitive translations $\mathbf{a}_i$, has a reciprocal cell based on the primitive translations $\mathbf{a}_i^*$. In reciprocal space, we may form the unique superlattices by means of the transformation:

$$\mathbf{b}_i^*=\textstyle\sum_j S_{ij}\mathbf{a}_j^*\,, \tag{11}$$

where the matrices $\mathbf{S}$ are those previously obtained. The reciprocal of a unique superlattice defined by the translations $\mathbf{b}_i^*$ is a unique sublattice defined by the

Table 1. *Unique matrices* $\mathbf{S}$ *generating superlattices for* $|\mathbf{S}|=2,3,4$

The unique matrices generating sublattices for $|\mathbf{S}|=\frac{1}{2},\frac{1}{3},\frac{1}{4}$ are obtained by taking the transpose of the inverse of the matrices given. For each value of $|\mathbf{S}|$, the matrices can be applied to any primitive cell of the original lattice, but they must be applied to the same cell.

Transformation matrix S	Conditions limiting the possible coordinates α_i of the superlattice nodes
	$\lvert\mathbf{S}\rvert=2$
200/010/001	$\alpha_1=2n$
100/020/001	$\alpha_2=2n$
100/010/002	$\alpha_3=2n$
200/110/001	$\alpha_1+\alpha_2=2n$
200/010/101	$\alpha_1+\alpha_3=2n$
100/011/002	$\alpha_2+\alpha_3=2n$
110/011/101	$\alpha_1+\alpha_2+\alpha_3=2n$
	$\lvert\mathbf{S}\rvert=3$
300/010/001	$\alpha_1=3n$
100/030/001	$\alpha_2=3n$
100/010/003	$\alpha_3=3n$
$1\bar{1}0/210/001$	$\alpha_1+\alpha_2=3n$
$110/\bar{2}10/001$	$\alpha_1-\alpha_2=3n$
$\bar{1}01/201/010$	$\alpha_1+\alpha_3=3n$
$101/20\bar{1}/010$	$\alpha_1-\alpha_3=3n$
$01\bar{1}/021/100$	$\alpha_2+\alpha_3=3n$
$011/0\bar{2}1/100$	$\alpha_2-\alpha_3=3n$
211/110/021	$-\alpha_1+\alpha_2+\alpha_3=3n$
$121/\bar{1}\bar{1}0/201$	$\alpha_1-\alpha_2+\alpha_3=3n$
112/101/210	$\alpha_1+\alpha_2-\alpha_3=3n$
111/120/021	$\alpha_1+\alpha_2+\alpha_3=3n$
	$\lvert\mathbf{S}\rvert=4$
400/010/001	$\alpha_1=4n$
100/040/001	$\alpha_2=4n$
100/010/004	$\alpha_3=4n$
400/310/001	$\alpha_1+\alpha_2=4n$
400/110/001	$\alpha_1-\alpha_2=4n$
400/010/301	$\alpha_1+\alpha_3=4n$
400/010/101	$\alpha_1-\alpha_3=4n$
100/013/004	$\alpha_2+\alpha_3=4n$
100/011/004	$\alpha_2-\alpha_3=4n$
400/210/001	$\alpha_1+2\alpha_2=4n$
400/010/201	$\alpha_1+2\alpha_3=4n$
100/021/002	$\alpha_2+2\alpha_3=4n$
200/120/001	$2\alpha_1+\alpha_2=4n$
200/010/102	$2\alpha_1+\alpha_3=4n$
100/012/004	$2\alpha_2+\alpha_3=4n$
220/011/101	$\alpha_1+\alpha_2-\alpha_3=4n$
110/011/202	$\alpha_1-\alpha_2+\alpha_3=4n$
110/022/101	$-\alpha_1+\alpha_2+\alpha_3=4n$
121/112/211	$\alpha_1+\alpha_2+\alpha_3=4n$
310/111/201	$\alpha_1+\alpha_2+2\alpha_3=4n$
400/110/201	$\alpha_1-\alpha_2+2\alpha_3=4n$
210/111/301	$\alpha_1+2\alpha_2+\alpha_3=4n$
400/210/101	$\alpha_1+2\alpha_2-\alpha_3=4n$
111/013/102	$2\alpha_1+\alpha_2+\alpha_3=4n$
200/011/102	$2\alpha_1+\alpha_2-\alpha_3=4n$
210/011/201	$\alpha_1+2\alpha_2+2\alpha_3=4n$
120/021/101	$2\alpha_1+\alpha_2+2\alpha_3=4n$
110/012/102	$2\alpha_1+2\alpha_2+\alpha_3=4n$
200/020/001	$\alpha_1=2n;\ \alpha_2=2m$
200/010/002	$\alpha_1=2n;\ \alpha_3=2m$
100/020/002	$\alpha_2=2n;\ \alpha_3=2m$
200/011/002	$\alpha_1=2n;\ \alpha_2+\alpha_3=2m$
200/020/101	$\alpha_2=2n;\ \alpha_1+\alpha_3=2m$
200/110/002	$\alpha_3=2n;\ \alpha_1+\alpha_2=2m$
200/111/002	$\alpha_1+\alpha_2=2n;\ \alpha_2+\alpha_3=2m$

translations $\mathbf{b}_i$ and given by:

$$\mathbf{b}_i = \sum_j T_{ji}\mathbf{a}_j \,. \tag{12}$$

Transformation (12) shows that, if **S** is a matrix that transforms the original lattice into a superlattice with determinant $|\mathbf{S}|$, then the transpose of matrix **T** is the matrix that transforms the original lattice into a sublattice with determinant $1/|\mathbf{S}|$. Matrices for obtaining sublattices with determinants $\frac{1}{2},\frac{1}{3},\frac{1}{4}$ can be obtained by taking the transpose of the inverse of the matrices reported in Table 1. As in the case of superlattices, each set of matrices generating sublattices must be applied to the same primitive cell of the original lattice, but the choice of this cell is arbitrary.

The transformation matrices needed for obtaining composite lattices from the original lattice can be found by multiplying, in any order and in any combination, matrices generating superlattices with matrices generating sublattices. Two simple examples of such matrices are

$$(100/020/001)\,.\,(\tfrac{1}{2}00/010/001) = (\tfrac{1}{2}00/020/001) \qquad |\mathbf{S}| = 1$$

and

$$(100/0\tfrac{1}{4}0/001)\,.\,(200/010/001) = (200/0\tfrac{1}{4}0/001) \qquad |\mathbf{S}| = \tfrac{1}{2}.$$

In the first example, the composite lattice is obtained by halving the $\mathbf{a}_1$ axis of the original cell and by doubling the $\mathbf{a}_2$ axis, and the determinant of the transformation is equal to one. In the second transformation, the $\mathbf{a}_1$ axis is doubled and the $\mathbf{a}_2$ axis is reduced to $\frac{1}{4}$ of the original length. The number of composite lattices that can be produced for any given value of the determinant of the transformation is unlimited. For example, composite lattices with $|\mathbf{S}| = 1$ can be obtained in a great variety of ways, such as by combining transformations with determinants 3 and $\frac{1}{3}$, or 2 and $\frac{1}{2}$, or 3, $\frac{1}{2}$, 2 and $\frac{1}{3}$, *etc.* So far we have made no attempt to classify these lattices or to determine their properties. Work on this subject, however, is planned.

References

Buerger, M. J. (1946). *J. Chem. Phys.* **15**, 1.

Buerger, M. J. (1954). *Proc. Nat. Acad. Sci. U.S.* **40**, 125.

Cassels, J. W. S. (1959). *An Introduction to the Geometry of Numbers*. New York: Springer Verlag.

Donnay, G., Donnay, J. D. H. & Kullerud, G. (1958). *Amer. Miner.* **43**, 228.

Friedel, G. (1964). *Leçons de Cristallographie*. Paris: Blanchard.

International Tables for X-ray Crystallography (1969). Vol. I. Birmingham: Kynoch Press.

Niggli, P. (1928). *Handbuch der Experimentalphysik*, Vol. 7, Part 1. Leipzig: Academische Verlagsgesellschaft.

Acta Cryst. (1972). A**28**, 287

The Resolution Function of a Slow Neutron Rotating-Crystal Time-of-Flight Spectrometer. II. Application to the Measurement of General Frequency Spectra

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The resolution function of a slow neutron rotating-crystal time-of-flight spectrometer applied to the measurement of general frequency spectra is treated analytically. It is demonstrated that every component of the instrument may contribute to the uncertainty of the time-of-flight measurement. Focusing conditions are derived, leading to the concept of removable and irremovable time-of-flight spreads. Experimental evidence is presented to support the resolution functions, calculated on the basis of this theory.

1. Introduction

In all neutron-scattering experiments, the observed spectra, $I(\mathbf{Q},\omega)$, are given by the convolution integral

$$I(\mathbf{Q},\omega) = \iint R(\mathbf{Q}'-\mathbf{Q},\omega'-\omega)\sigma(\mathbf{Q}',\omega')\mathrm{d}\mathbf{Q}'\mathrm{d}\omega', \tag{1.1}$$

where $R(\mathbf{Q},\omega)$ is the instrumental resolution function and $\sigma(\mathbf{Q},\omega)$ is the unknown scattering cross section. $\mathbf{Q}$ and ω are defined by the momentum transfer:

$$\hbar\mathbf{Q} = \hbar(\mathbf{k}_{12}-\mathbf{k}_{23})\,, \tag{1.2}$$

and by the energy transfer:

$$\hbar\omega = \frac{\hbar^2}{2m}(\mathbf{k}_{12}^2-\mathbf{k}_{23}^2)\,, \tag{1.3}$$

in which m denotes the neutron mass. The indices 0, 1, 2, 3 refer to the different spectrometer elements,