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Commission on Crystallographic Nomenclature
International Union of Crystallography

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Crystallography (IUCr Commission)

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Detailed Licensing

Detailed Licensing

Licensing

A detailed breakdown of this resource's licensing can be found in ***Back Matter/Detailed Licensing****.*

CHAPTER OVERVIEW

1: Fundamental Crystallography

1.1: Abelian group

An **abelian group**, also called a *commutative group*, is a group (G, *) such that

$$g_1 * g_2 = g_2 * g_1$$

for all g_1 and g_2 in G, where $*$ is a binary operation in G. This means that the order in which the binary operation is performed does not matter, and any two elements of the group commute.

Groups that are not commutative are called **non-abelian** (rather than non-commutative).

Abelian groups are named after Niels Henrik Abel.

1.2: Absolute structure

The spatial arrangement of the atoms of a physically identified non-centrosymmetric crystal and its description by way of unit-cell dimensions, space group, and representative coordinates of all atoms.

1.3: Affine Isomorphism

Each symmetry operation of crystallographic group in E^3 may be represented by a 3×3 matrix **W** (the *linear part*) and a vector **w**. Two crystallographic groups $G_1 = \{(\mathbf{W}_{1i},\mathbf{w}_{1i})\}$ and $G_2 = \{(\mathbf{W}_{2i},\mathbf{w}_{2i})\}$ are called **affine isomorphic** is there exists a non-singular 3×3 matrix **A** and a vector **a** such that:

$$G_2 = \{(\mathbf{A},\mathbf{a})(\mathbf{W}_{1i},\mathbf{w}_{1i})(\mathbf{A},\mathbf{a})^{-1}\}$$

Two crystallographic groups are affine isomorphic if and only if their arrangement of symmetry elements may be mapped onto each other by an affine mapping of E^3. Two affine isomorphic groups are always isomorphic.

1.4: Affine mapping

An **affine mapping** is any mapping that preserves collinearity and ratios of distances: if three points belong to the same straight line, their images under an affine transformation also belong to the same line. Moreover, the middle point is also conserved under the affine mapping. By contrast, angles and lengths in general are not kept constant by an affine mapping.

Under an affine mapping:

- parallel lines remain parallel;
- concurrent lines remain concurrent (images of intersecting lines intersect);
- the ratio of length of segments of a given line remains constant;
- the ratio of areas of two triangles remains constant;
- ellipses, parabolas and hyperbolas remain ellipses, parabolas and hyperbolas respectively;
- barycenters of polygons map into the corresponding barycenters.

Geometric contraction, expansion, dilation, reflection, rotation, shear, similarity transformations, spiral similarities, and translation are all affine transformations, as are their combinations. Affine mappings that keep also distances and angles are called Euclidean mappings.

1.5: Aperiodic crystal

A *periodic crystal* is a structure with, ideally, sharp diffraction peaks on the positions of a *reciprocal lattice*. The structure then is invariant under the translations of the *direct lattice*. Periodicity here means *lattice periodicity*. Any structure without this property is *aperiodic*. For example, an amorphous system is aperiodic. An *aperiodic crystal* is a structure with sharp diffraction peaks, but without lattice periodicity. Therefore, amorphous systems are not aperiodic crystals. The positions of the sharp diffraction peaks of an aperiodic crystal belong to a *vector module* of finite rank. This means that the diffraction wave vectors are of the form

$$\mathbf{k} = \sum_{i-1}^{n} h_i \mathbf{a}_i^*, (integer\, h_i)$$

The basis vectors a_i^* are supposed to be independent over the rational numbers, i.e. when a linear combination of them with rational coefficients is zero, all coefficients are zero. The minimum number of basis vectors is the *rank* of the vector module. If the rank *n* is larger than the space dimension, the structure is not periodic, but aperiodic.

1.6: Aristotype

An aristotype is a high-symmetry structure type that can be viewed as an idealized version of a lower-symmetry structure. It was introduced by Helen Megaw in relation to perovskites, where it is still mostly used. The cubic perovskite structure (which is adopted at most by half a dozen compounds) is regarded as the aristotype for the vast array of other lower-symmetry perovskites. The lower-symmetry structure is called **hettotype**.

After Buerger, aristotypes are also known as **basic structures** and hettotypes as **derivative structures**.

Originally, an aristotype is a printing-out process using paper coated with silver chloride in gelatin; now, any such process using silver salts in either collodion or gelatin; also, a print so made.

1.7: Arithmetic crystal class

The **arithmetic crystal classes** are obtained in an elementary fashion by combining the geometric crystal classes and the corresponding types of Bravais lattices. For instance, in the monoclinic system, there are three geometric crystal classes, 2, *m* and 2/*m*, and two types of Bravais lattices, *P* and *C*. There are therefore six monoclinic arithmetic crystal classes. Their symbols are obtained by juxtaposing the symbol of the geometric class and that of the Bravais lattice, in that order: 2*P*, 2*C*, *mP*, *mC*, 2/*mP*, 2/*mC* (note that in the space group symbol the order is inversed: *P*2, *C*2, etc...). In some cases, the centering vectors of the Bravais lattice and some symmetry elements of the crystal class may or may not be parallel; for instance, in the geometric crystal class *mm* with the Bravais lattice *C*, the centering vector and the two-fold axis may be perpendicular or coplanar, giving rise to two different arithmetic crystal classes, *mm*2*C* and 2*mmC* (or *mm*2*A*, since it is usual to orient the two-fold axis parallel to *c*), respectively. There are 13 two-dimensional arithmetic crystal classes and 73 three-dimensional arithmetic crystal classes that are listed in the attached **table**. Space groups belonging to the same geometric crystal class and with the same type of Bravais lattice belong to the same arithmetic crystal class; these are therefore in one to one correspondence with the symmorphic space groups.

The group-theoretical definition of the arithmetic crystal classes is given in Section 8.2.3 of *International Tables of Crystallography, Volume A*.

1.8: Asymmetric Unit

An asymmetric unit of a space group is a simply connected smallest closed part of space from which, by application of all symmetry operations of the space group, the whole space is filled. This implies that:

- mirror planes must form boundary planes of the asymmetric unit;
- rotation axes must form boundary edges of the asymmetric unit;
- inversion centers must either form vertices of the asymmetric unit or be located at the midpoints of boundary planes or boundary edges.

These restrictions do not hold for screw axes and glide planes.

The term "asymmetric unit" does not mean that this region has an asymmetric shape. In mathematics it is called fundamental region or fundamental domain.

1.9: Automorphism

An isomorphism from a group $(G,*)$ to itself is called an **automorphism** of this group. It is a bijection $f: G \rightarrow G$ such that

$$f(g) * f(h) = f(g * h)$$

An automorphism preserves the structural properties of a group, e.g.:

- The identity element of G is mapped to itself.
- Subgroups are mapped to subgroups, normal subgroups to normal subgroups.
- Conjugacy classes are mapped to conjugacy classes (the same or another).
- The image $f(g)$ of an element g has the same order as g.

The composition of two automorphisms is again an automorphism, and with composition as binary operation the set of all automorphisms of a group G, denoted by **Aut(*G*)**, forms itself a group, the *automorphism group* of G.

1.10: Binary Operation

A **binary operation** on a set S is a mapping f from the Cartesian product $S \times S$ to S. A mapping from K x S to S, where K need not be S, is called an **external binary operation**.

Many binary operations are commutative (i.e. $f(a,b) = f(b,a)$ holds for all a, b in S) or associative (i.e. $f(f(a,b), c) = f(a, f(b,c))$ holds for all a,b,c in S). Many also have identity elements and inverse elements. Typical examples of binary operations are the addition (+) and multiplication (*) of numbers and matrices as well as composition of functions or symmetry operations.

Examples of binary operations that are not commutative are subtraction (-), division (/), exponentiation(^), super-exponentiation(@), and composition.

Binary operations are often written using infix notation such as $a * b$, $a + b$, or $a \cdot b$ rather than by functional notation of the form $f(a,b)$. Sometimes they are even written just by concatenation: ab.

1.100: Subperiodic group

A **subperiodic group** is a group of Euclidean mappings such that its translations form a lattice in a proper subspace of the space on which it acts.

A **crystallographic subperiodic group** in n-dimensional space is a subperiodic group for which the group of linear parts is a crystallographic point group of n-dimensional space. The crystallographic subperiodic groups in two and three-dimensional space are classified in:

- **frieze groups**: 7 two-dimensional groups with one-dimensional translations;
- **rod groups**: 75 three-dimensional groups with one-dimensional translations;
- **layer groups**: 80 three-dimensional groups with two-dimensional translations.

1.101: Supercell

A cell C' obtained from a cell C by removing one or more translation vectors is called a **supercell** of C. The translation subgroup **T'** of the lattice **L'** built on C' is a subgroup of the translation subgroup **T** of the lattice **L** built on C and corresponds therefore to sublattice of **L**.

Contributors

1.102: Supergroup

If G is a group and H is a subgroup of G, then G is a **supergroup** of H.

If H is a maximal subgroup of G, then G is a **minimal supergroup** of H.

1.103: Superlattice

A lattice **L'** obtained by another lattice **L** by adding one or more sets of nodes is called a **superlattice of L**. The translation subgroup **T'** of **L'** is a supergroup of the translation subgroup **T** of **L**. The unit cell of **L'** is smaller than the unit cell of **L** and is therefore called a subcell.

1.104: Symmetry element

A **symmetry element** (of a given crystal structure or object) is defined as a concept with a double meaning, namely the combination of a geometric element with the set of symmetry operations having this geometric element in common (termed its *element set*). Together with the identity and the translations, for which a geometric element is not defined, the element sets cover all symmetry operations.

1.105: Symmetry operation

A **symmetry operation** is an **isometry**, *i.e.* a transformation under which two objects, or two configurations or an object, are brought to coincide. A symmetry operation is a Euclidean mapping: to each point of the first configuration there corresponds a point of the second configuration, the distances between two points are kept by the transformation, as are the angles.

The two configurations/objects can be either congruent or enantiomorphous. Correspondingly, the symmetry operations are classed into two kinds:

- **symmetry operations of first kind**: they relate congruent objects and consist of translations, rotations and screw rotations;
- **symmetry operations of second kind**: they relate enantiomorphous objects and consist of inversion, reflections, rotoinversions, and glide reflections. There exist a 1:1 correspondence between rotoinversion and rotoreflections: the latter are more used in Schoenflies notation, whereas rotoinversions are preferred in Hermann-Mauguin notation.

A symmetry operation is performed about a symmetry element.

1.106: Symmorphic space groups

A space group is called ‘symmorphic’ if, apart from the lattice translations, all generating symmetry operations leave one common point fixed. Permitted as generators are thus only the point-group operations: rotations, reflections, inversions and rotoinversions. The symmorphic space groups may be easily identified because their Hermann-Mauguin symbol does not contain a glide or screw operation. The combination of the Bravais lattices with symmetry elements with no translational components yields the 73 symmorphic space groups, *e.g.* *P*2, *Cm*, *P*2/*m*, *P*222, *P*32, *P*23. They are in one to one correspondence with the arithmetic crystal classes.

A characteristic feature of a symmorphic space group is the existence of a special position, the site-symmetry group of which is isomorphic to the point group to which the space group belongs. Symmorphic space groups have no zonal or serial reflection conditions, but may have integral reflection conditions (*e.g.* *C*2, *Fmmm*).

1.107: Tetartohedry

The point group of a crystal is called tetartohedry if it is a subgroup of index 4 of the point group of its lattice.

1.108: Unit cell

The **unit cell** is the parallelepiped built on the vectors, **a**, **b**, **c**, of a crystallographic basis of the direct lattice. Its volume is given by the scalar triple product, $V = (\mathbf{a}, \mathbf{b}, \mathbf{c})$ and corresponds to the square root of the determinant of the metric tensor.

If the basis is primitive, the unit cell is called the primitive cell. It contains only one lattice point. If the basis is non-primitive, the unit cell is a multiple cell and it contains more than one lattice point. The multiplicity of the cell is given by the ratio of its volume to the volume of a primitive cell.

1.109: Vector module

A *vector module* is the set of vectors spanned by a number n of basis vectors with integer coefficients. The basis vectors should be independent over the integers, which means that any linear combination

$$\sum_{i} m_i a_i$$

with m_i integers is equal to zero if, and only if, all coefficients m_i are zero. The term Z-module is sometimes used to underline the condition that the coefficients are integers. The number of basis vectors is the *rank* of the vector module.

1.11: Bragg's Law

Bragg's law provides the condition for a plane wave to be diffracted by a family of lattice planes:

$$2d\sin\theta = n\lambda.$$

where d is the **lattice** spacing, θ the angle between the wavevector of the incident plane wave, $\mathbf{k_o}$, and the lattice planes, λ its wave length and n is an integer, the order of the reflection. It is equivalent to the diffraction condition in reciprocal space and to the Laue equations.

Direct Derivation of Bragg's Law

- **Reflection from the first plane:** The scattered waves will be in phase whatever the distribution of the point scatterers in the first plane if the angle of the reflected wave vector, $\mathbf{k_h}$, is also equal to θ. This is Snell-Descartes' law of reflection.
- **Reflection from the second plane:** Since the phase of the reflected waves is independent of the position of the point scatterer in the plane, the phase difference between the waves reflected by two successive lattice planes is obtained by choosing arbitrarily a scattering point, *A*, on the first plane and a scattering point, *b* on the second plane such that *AB* is normal to the planes. If *C* and *d* are the projections of *A* on the incident and reflected wave vectors passing through *B*, it is clear from Figure 1 that the path difference between the waves reflected at *A* and *B*, respectively, is:

  $$CB + BD = 2d\sin\theta$$

  and that the two waves will be in phase if this path difference is equal to $n\,\lambda$ where n is an integer.
- **Reflection from the third, etc., planes:** If Bragg's relation is satisfied for the first two planes, the waves reflected with wave vector $\mathbf{k_h}$ will be in phase fo all the planes of the family.

Order of the Reflection

Bragg's law may also be written:

$$2(d/n)sin\theta = \lambda.$$

One may then say that a Bragg reflection of order n on a family of lattice planes or order n is equivalent to reflection of order 1 on a family of fictitious, or imaginary, planes of lattice spacing:

$$d_{hkl} = \frac{d}{n}$$

This fictitious family is associated to the reciprocal lattice vector **OH** where $OH = n/d = 1/d_{hkl}$. The indices of the reflection are:*hkl*. For instance, the dashed blue lines in Figure 1 correspond to the fistitious planes associated to the second order, $n = 2$.

Extinctions or Systematic Absences

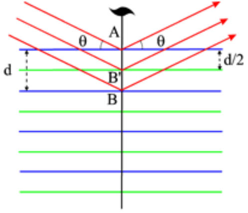

Figure 2

If there is a glide plane or a screw axis normal to the lattice planes, the spacing of the actual reflecting planes is $d/2$ for a glide plane and $(d\,p/q)$ for a q_p screw axis. Bragg's law should then be written:

$$2\left(\frac{d}{2}\right)\sin\theta = n\lambda$$

$$2d\sin\theta = 2n\lambda$$

for a glide plane and

$$2(dp/q)\sin\theta = n\lambda \Rightarrow 2d\sin\theta = (q/p)n\lambda$$

for a screw axis q_p.

The reflections of odd order for a glide plane and of order different from (q/p)n for a screw axis are then absent. One speaks of extinctions or systematic absences related to the presence of glide or screw components.

As an example, Figure 2 shows the case of a 2_1 screw axis: the reflecting planes are the blue planes and the green planes deduced from the latter by the action of the screw axis. Reflections of odd order will be sytematically absent.

Influence of deformation

A deformation that leaves a family of lattice planes (*hkl*) undistorted and its lattice spacing *d* unchanged will not affect the Bragg angle of *kkl* reflections, *e.g.* lattice planes parallel to a screw dislocations.

History

Bragg (1890-1971) presented his derivation of the reflection condition at a meeting of the Cambridge Philosophical Society on 11 November 1912. His paper was published in 1913 (Bragg W.L., 1913, *The Diffraction of Short Electromagnetic Waves by a Crystal*, *Proc. Cambridge Phil. Soc.*, **17**, 43-57. For details, see P. P. Ewald, 1962, IUCr, 50 Years of X-ray Diffraction, Section 5, page 64.

1.110: Vector space

For each pair of points X and Y in point space one can draw a vector **r** from X to Y. The set of all vectors forms a **vector space**. The vector space has no origin but instead there is the *zero vector* which is obtained by connecting any point X with itself. The vector **r** has a *length* which is designed by |**r**| = r, where r is a non–negative real number. This number is also called the *absolute value* of the vector. The maximal number of linearly independent vectors in a vector space is called the *dimension of the space*.

An essential difference between the behavior of vectors and points is provided by the changes in their coefficients and coordinates if a different origin in point space is chosen. The coordinates of the points change when moving from an origin to the other one. However, the coefficients of the vector **r** do not change.

The point space is a dual of the vector space because to each vector in vector space a pair of points in point space can be associated.

Face normals, translation vectors, Patterson vectors and reciprocal lattice vectors are elements of vector space.

1.111: Voronoi domain

The Voronoi domain (or 'cell', or 'region') is the name given in mathematics to the Wigner-Seitz cell. Voronoi domains are in the form of polyhedra and are classified according to their topological properties ; one distinguishes five types of Voronoi polyhedra (see Section 9.1.6 of *International Tables of Crystallography, Volume A*.

1.112: Weissenberg complex

A **Weissenberg complex** is a lattice complex for which the multiplicity does not decrease for any special values of the coordinates. Weissenberg complexes can simulate invariant lattice complexes as limiting complexes.

1.113: Wigner-Seitz cell

The Wigner-Seitz cell is a a polyhedron obtained by connecting a lattice point *P* to all other lattice points and drawing the planes perpendicular to these connecting lines and passing through their midpoints (Figure 1). The polyhedron enclosed by these planes is the Wigner-Seitz cell. This construction is called the *Dirichlet* construction. The cell thus obtained is a primitive cell and it is possible to fill up the whole space by translation of that cell.

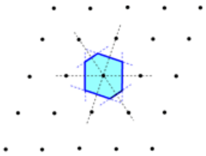

Figure 1 Wigner-Seitz cell.
Shaded: domain of influence.

The Wigner-Seitz cell of a body-centered cubic lattice *I* is a cuboctahedron (Figure 2) and the Wigner-Seitz cell of a face-centered cubic lattice *F* is a rhomb-dodecahedron (Figure 3). In reciprocal space this cell is the first Brillouin zone. Since the reciprocal lattice of body-centered lattice is a face-centered lattice and reciprocally, the first Brillouin zone of a body-centered cubic lattice is a rhomb-dodecahedron and that of a face-centered cubic lattice is a cuboctahedron.

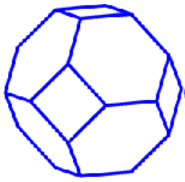

Figure 2.

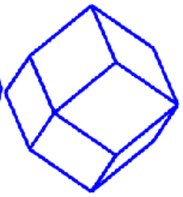

Figure 3.

The inside of the Wigner-Seitz cell has been called domain of influence by Delaunay (1933). It is also called Dirichlet domain or Voronoi domain. The domain of influence of lattice point *P* thus consists of all points *Q* in space that are closer to this lattice point than to any other lattice point or at most equidistant to it (such that $\mathbf{OP} \leq |\mathbf{t} - \mathbf{OP}|$ for any vector $\mathbf{t} \in L$).

1.114: Wyckoff position

A **Wyckoff position** of a space group G consists of all points *X* for which the site-symmetry groups are conjugate subgroups of G.

Each Wyckoff positon of a space group is labeled by a letter which is called the *Wyckoff letter*.

The number of different Wyckoff positions of each space group is finite, the maximal numbers being 9 for plane groups (realized in *p*2*mm*) and 27 for space groups (realized in *Pmmm*).

There is a total of 72 Wyckoff positions in plane groups and 1731 Wyckoff positions in space groups.

The transfer of Wyckoff positions from individual space groups to space-group types is not unique because Wyckoff positions with the same type of site-symmetry group may be exchanged in different space groups of the same type. This is no longer true when one makes use of Wyckoff sets.

1.115: Wyckoff set

A *Wyckoff set* with respect to a space group G is the set of all points X for which the site-symmetry groups are conjugate subgroups of the normalizer N of G in the group of all affine mappings.

Any Wyckoff position of G is transformed onto itself by all elements of G, but not necessarily by the elements of N. Any Wyckoff set of G is instead transformed onto itself also by those elements of N that are contained in G.

1.12: Bravais-Miller indices

The Bravais-Miller indices are used in the case of hexagonal lattices. In that case, one uses four axes, $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$, $\mathbf{c}$ and four Miller indices, ($hkil$), where h, k, i, l are prime integers inversely proportional to the intercepts OP, OQ, OS, OR of a plane of the family with the four axes. The indices h, k, i are cyclically permutable and related by $h + k + i = 0$

1.13: Bravais class

An arithmetic crystal class with matrix group of lattices is called a *Bravais arithmetic crystal class*, or **Bravais class** for short.

Each lattice is associated with a Bravais class, and each matrix group of a Bravais class represents the point group of a lattice referred to an appropriate primitive basis.

There exist 5 Bravais classes in two dimensions:

- $2p$
- $2mmp$
- $2mmc$
- $4mmp$
- $6mmh$

There exist 14 Bravais classes in three dimensions:

- $\bar{1}P$
- $2/mP$
- $2/mS$
- $mmmP$
- $mmmS$
- $mmmI$
- $mmmF$
- $4/mmmP$
- $4/mmmI$
- $\bar{3}mR$
- $6/mmmP$
- $m\bar{3}mP$
- $m\bar{3}mI$
- $m\bar{3}mF$

1.14: Bravais flock

Space groups that are assigned to the same Bravais class belong to the same **Bravais flock of space groups**.

The introduction of the concept of Bravais flock is necessary in order to classify space groups on the basis of their Bravais type of lattice, independently from any accidental metric of the lattice.

An orthorhombic crystal may have accidentally $a = b$ have a tetragonal lattice not because of symmetry restrictions but just by accident. If the Bravais types of lattices were used directly to classify space group, such a crystal would be go in another category with respect to an orthorhombic crystal without specialized metric. The concept of Bravais flock solves this ambiguity.

A space group G is *assigned* to a Bravais class on the basis of the corresponding point group P and the arithmetic crystal class associated with it:

- If the arithmetic crystal class of G is a Bravais class, then G is assigned to that Bravais class;
- if the arithmetic crystal class of G is not a Bravais class, then the Bravais class to which G is assigned is obtained as follows:
  - those Bravais classes are retained whose point group B is such that P is a subgroup of B;
  - G is assigned to that Bravais class, among those selected above, for which the ratio of the order of the point groups of B and of P is minimal.

For example, a space group of type $I4_1$ belongs to the arithmetic crystal class $4I$, to which two Bravais class can be associated, $4/mmmI$ and $m\bar{3}mI$. The second condition uniquely assigns G to the Bravais flock of $4/mmmI$, despite the fact that the Bravais class of the lattice may be $m\bar{3}mI$ as a result of accidental symmetry.

1.15: Bravais lattice

The current nomenclature adopted by the IUCr prefers to use the expression **Bravais types of lattices** to emphasize that **Bravais lattices** are not individual lattices but types or classes of all lattices with certain common properties .

All vector lattices whose matrix groups belong to the same Bravais class correspond to the same **Bravais type of lattice**.

1.16: Brillouin zones

A *Brillouin Zone* is a particular choice of the unit cell of the reciprocal lattice. It is defined as the Wigner-Seitz cell (also called *Dirichlet* or *Voronoi Domain*) of the reciprocal lattice. It is constructed as the set of points enclosed by the *Bragg planes*, the planes perpendicular to a connection line from the origin to each lattice point and passing through the midpoint. Alternatively, it is defined as the set of points closer to the origin than to any other reciprocal lattice point. The whole reciprocal space may be covered without overlap with copies of such a Brillouin Zone.

For high-symmetry lattices one introduces sometimes the notion of *n-th Brillouin Zone*. This is the set of points one reaches with a straight line from the origin and passing through *n*-1 Bragg Planes. In this terminology, the Brillouin Zone defined above is the first Brillouin Zone. The *n*-th Brillouin Zone is a shell around lower Brillouin Zones and its shape becomes for higher values of *n* rapidly rather complicated.

Vectors in the Brillouin Zone or on its boundary characterize states in a system with lattice periodicity, e.g. phonon or electron states. States are non-equivalent if they belong to different vectors in a unit cell of the reciprocal lattice. This is not necessarily the Brillouin Zone. Especially, for low-symmetry systems Brillouin Zones are sometimes difficult to visualize, and another choice of unit cell may be useful, e.g. the parallelepiped spanned by the basis vectors.

The Brillouin Zone boundary consists of pieces of Bragg planes. Since two points on the boundary may differ by a reciprocal lattice vector, only a part of the boundary may be used for characterization of states. There is no simple rule for that choice. Dispersion curves at the zone boundary have either a maximum or minimum there or they merge with other curves giving rise to a change of degeneracy.

See also

Section 2.2 of *International Tables of Crystallography, Volume D*

1.17: Cartesian product

The **Cartesian product** is a direct product of sets.

The Cartesian product of two sets X and Y, denoted $X \times Y$, is the set of all possible ordered pairs whose first component is a member of X and whose second component is a member of Y:

$$X \times Y = \{(x,y) | x \in X \text{ and } y \in Y\}.$$

A Cartesian product of two finite sets can be represented by a table, with one set as the rows and the other as the columns, and forming the ordered pairs, the cells of the table, by choosing the element of the set from the row and the column.

1.18: Center

The **center** (or **centre**) of a group G is the set $Z(G) = \{ a \text{ in } G : a*g = g*a \text{ for all } g \text{ in } G \}$ of elements commuting with all elements of G. The center is an Abelian group.

The center of a group G is always a normal subgroup of G, namely the kernel of the homomorphism mapping an element a of G to the inner automorphism $f_a: g \rightarrow aga^{-1}$.

1.19: Centered lattices

When the unit cell does not reflect the symmetry of the lattice, it is usual in crystallography to refer to a 'conventional', non-primitive, crystallographic basis, $\mathbf{a_c}$, $\mathbf{b_c}$, $\mathbf{c_c}$ instead of a primitive basis, **a**, **b**, **c**. This is done by adding lattice nodes at the center of the unit cell or at one or three faces. The vectors joining the origin of the unit cell to these additional nodes are called 'centering vectors'. In such a lattice $\mathbf{a_c}$, $\mathbf{b_c}$ and $\mathbf{c_c}$ with all their integral linear combinations are lattice vectors again, but there exist other lattice vectors $\mathbf{t} \in \mathbf{L}$, $\mathbf{t} = t_1\, \mathbf{a_c} + t_2\, \mathbf{b_c} + t_3\, \mathbf{c_c}$; with at least two of the coefficients t_1, t_2, t_3 being fractional. The table below gives the various types of centering vectors and the corresponding types of centering. Each one is described by a letter, called the Bravais letter, which is to be found in the Hermann-Mauguin symbol of a space group.

The 'multiplicity', m, of the centered cell is the number of lattice nodes per unit cell (see table).

The volume of the unit cell, $V_c = (\mathbf{a_c}, \mathbf{b_c}, \mathbf{c_c})$ is given in terms of the volume of the primitive cell, $V = (\mathbf{a}, \mathbf{b}, \mathbf{c})$, by:

$V_c = m\, V$

1.20: Centralizer

The **centralizer** $C_G(g)$ of an element g of a group G is the set of elements of G which commute with g:

$$C_G(g) = \{x \in G : xg = gx\}.$$

If H is a subgroup of G, then $C_H(g) = C_G(g) \cap H$.

More generally, if S is any subset of G (not necessarily a subgroup), the centralizer of S in G is defined as

$$C_G(S) = \{x \in G : \forall\ s \in S, xs = sx\}.$$

If S = {g}, then C(S) = C(g).

C(S) is a subgroup of G; in fact, if x, y are in C(S), then $xy^{-1}s = xsy^{-1} = sxy^{-1}$.

1.21: Complex

A **complex** is a subset obtained from a group by choosing part of its elements in such a way that the closure property of groups is not respected. Therefore, a complex is not a group itself.

A typical example of complexes is that of cosets. In fact, a coset does not contain the identity and therefore it is not a group.

A subgroup is a particular case of complex that obeys the closure property and is a group itself.

1.22: Conjugacy class

If g_1 and g_2 are two elements of a group G, they are called **conjugate** if there exists an element g_3 in G such that:

$$g_3 g_1 g_3^{-1} = g_2.$$

Conjugacy is an equivalence relation and therefore partitions G into equivalence classes: every element of the group belongs to precisely one conjugacy class

The equivalence class that contains the element g_1 in G is

$$Cl(g_1) = \{ g_3 g_1 g_3^{-1} | \ g_3 \in G\}$$

and is called the **conjugacy class** of g_1. The **class number** of G is the number of conjugacy classes.

The classes $Cl(g_1)$ and $Cl(g_2)$ are equal if and only if g_1 and g_2 are conjugate, and disjoint otherwise.

For Abelian groups the concept is trivial, since each element forms a class on its own.

1.23: Conventional cell

For each lattice, the **conventional cell** is the cell obeying the following conditions:

- its basis vectors define a right-handed axial setting;
- its edges are along symmetry directions of the lattice;
- it is the smallest cell compatible with the above condition.

Crystals having the same type of conventional cell belong to the same crystal family.

1.24: Coset

If G is a group, H a subgroup of G, and g an element of G, then

gH = { gh : h ∈ H } is a **left coset of H** in *G*
Hg = { hg : h ∈ H } is a **right coset of H** in *G*.

The decomposition of a group into cosets is unique. Left coset and right cosets however in general do not coincide, unless H is a normal subgroup of G.

Any two left cosets are either identical or disjoint: the left cosets form a partition of G, because every element of G belongs to one and only one left coset. In particular the identity is only in one coset, and that coset is H itself; this is also the only coset that is a subgroup. The same holds for right cosets.

All left cosets and all right cosets have the same order (number of elements, or cardinality), equal to the order of H, because H is itself a coset. Furthermore, the number of left cosets is equal to the number of right cosets and is known as the **index** of H in G, written as [G : H] and given by Lagrange's theorem:

|G|/|H| = [G : H].

Cosets are also sometimes called *associate complexes*.

Example

The coset decomposition of the twin lattice point group with respect to the point group of the individual gives the different possible twin laws. Each element in a coset is a possible twin operation.

Contributors

1.25: Crystal

Those solids in which atoms, ions or molecules are arranged in a definite three dimensional pattern are called crystalline solids. A material is a crystal if it has **essentially** a sharp diffraction pattern. The word **essentially** means that most of the intensity of the diffraction is concentrated in relatively sharp **Bragg peaks**, besides the always present diffuse scattering. In all cases, the positions of the diffraction peaks can be expressed by

$$H = \sum_{i=1}^{n} h_i a_i^* \ (n \geq 3)$$

Here $\mathbf{a}_i^*$ and h_i are the basis vectors of the reciprocal lattice and integer coefficients respectively and the number $n \backslash 0 istheminimumforwhichthepositionsofthepeakscanbedescribedwithintegercoefficient \backslash (h_i$. The conventional crystals are a special class, though very large, for which $n = 3$.

See also

Acta Cryst. (1992), **A48**, 928 where the definition of a crystal appears in the **Terms of reference** of the IUCr commission on aperiodic crystals

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  - Online Dictionary of Crystallography

1.26: Crystallographic basis

A basis of n vectors $\mathbf{e_1}$, $\mathbf{e_2}$, ... , $\mathbf{e_n}$ of the vector space $\mathbf{V^n}$ is a *crystallographic basis* of the vector lattice **L** if *every* integral linear combination $\mathbf{t} = u^1\mathbf{e_1} + u^2\mathbf{e_2} + ... + u^n\mathbf{e_n}$ is a lattice vector of **L**. It may or may not be a primitive basis.

1.27: Crystallographic orbit

In mathematics , an *orbit* is a general group-theoretical term describing any set of objects that are mapped onto each other by the action of a group. In crystallography, the concept of orbit is used to indicate a point configuration in association with its generating group.

From any point of the three-dimensional Euclidean space the symmetry operations of a given space group G generate an infinite set of points, called a **crystallographic orbit**. The space group G is called the **generating space group** of the orbit. Two crystallographic orbits are said configuration-equivalent if and only if their sets of points are identical.

1.28: Crystallographic symmetry

A motion is called a **crystallographic symmetry operation** if a crystal pattern exists for which it is a symmetry operation.

1.29: Crystal family

A **crystal family** is the smallest set of space groups containing, for any of its members, all space groups of the Bravais flock and all space groups of the geometric crystal class to which this member belongs.

1.30: Crystal pattern

An object in the n-dimensional point space E^n is called an n-dimensional **crystallographic pattern** or, for short, **crystal pattern** if among its symmetry operations:

1. there are *n* translations, the translation vectors $\mathbf{t}_1, \ldots, \mathbf{t}_n$ of which are linearly independent;
2. all translation vectors, except the zero vector **0**, have a length of at least $d > 0$.

When the crystal pattern consists of atoms, it takes the name of **crystal structure**. The crystal pattern is thus the generalization of a crystal structure to any pattern, concrete of abstract, in any dimension, which obeys the conditions of periodicity and discreteness expressed above.

1.31: Crystal system

A crystal-class system , or **crystal system** for short, contains complete geometric crystal classes of space groups . All those geometric crystal classes belong to the the same crystal system which intersect exactly the same set of Bravais flocks.

1.32: Direct Lattice

The direct lattice represents the triple periodicity of the ideal infinite perfect periodic structure that can be associated to the structure of a finite real crystal. To express this periodicity one calls *crystal pattern* an object in point space E^n (direct space) that is invariant with respect to three linearly independent translations, $\mathbf{t_1}$, $\mathbf{t_2}$ and $\mathbf{t_3}$. One distinguishes two kinds of lattices, the *vector lattices* and the *point lattices*.

Any translation $\mathbf{t} = u^i\,\mathbf{t_i}$ (u^i arbitrary integers) is also a translation of the pattern and the infinite set of all translation vectors of a crystal pattern is the **vector lattice L** of this crystal pattern.

Given an arbitrary point P in point space, the set of all the points P_i deduced from one of them by a translation $\mathbf{PP_i} = \mathbf{t_i}$ of the vector lattice **L** is called the **point lattice**.

A basis **a**, **b**, **c** of the vector space $\mathbf{V^n}$ is a *crystallographic basis* of the vector lattice **L** if *every* integral linear combination $\mathbf{t} = u\,\mathbf{a} + v\,\mathbf{b} + w\,\mathbf{c}$ is a lattice vector of **L**. It is called a *primitive basis* if *every* lattice vector **t** of **L** may be obtained as an integral linear combination of the basis vectors, **a**, **b**, **c**. Referred to any crystallographic basis the coefficients of each lattice vector are either integral or rational, while in the case of a primitive basis they are integral. *Non-primitive* bases are used conventionally to describe *centered lattices*.

The parallelepiped built on the basis vectors is the *unit cell*. Its volume is given by the triple scalar product, $V = (\mathbf{a}, \mathbf{b}, \mathbf{c})$.

If the basis is primitive, the unit cell is called the *primitive cell*. It contains only one lattice point. If the basis is non-primitive, the unit cell is a *multiple cell* and it contains more than one lattice point. The multiplicity of the cell is given by the ratio of its volume to the volume of a primitive cell.

The generalization of the notion of point and vector lattices to *n*-dimensional space is given in Section 8.1 of *International Tables of Crystallography, Volume A*

1.33: Direct product

In group theory, **direct product** of two groups (G, *) and (H, o), denoted by $G \times H$ is the as set of the elements obtained by taking the cartesian product of the sets of elements of G and H: {(g, h): g in G, h in H};

For abelian groups which are written additively, it may also be called the *direct sum* of two groups, denoted by $G \oplus H$.

The group obtained in this way has a normal subgroup isomorphic to G (given by the elements of the form (g, 1)), and one isomorphic to H (comprising the elements (1, h)).

The reverse also holds: if a group K contains two normal subgroups G and H, such that $K= GH$ and the intersection of G and H contains only the identity, then $K = G$ x H. A relaxation of these conditions gives the semidirect product.

1.34: Direct space

The direct space (or *crystal space*) is the *point space*, E^n, in which the structures of finite real crystals are idealized as infinite perfect three-dimensional structures. To this space one associates the *vector space*, V^n, of which lattice and translation vectors are elements. It is a *Euclidean* space where the scalar product of two vectors is defined. The two spaces are connected through the following relations:

(i) To any two points P and Q of the point space E^n a vector $\mathbf{PQ} = \mathbf{r}$ of the vector space V^n is attached

(ii) For each point P of E^n and for each vector $\mathbf{r}$ of V^n there is exactly one point Q of E^n for which $\mathbf{PQ} = \mathbf{r}$ holds

(iii) If R is a third point of the point space, $\mathbf{PQ} + \mathbf{QR} = \mathbf{PR}$

1.35: Displacive modulation

For a *displacively modulated crystal phase*, the positions of the atoms are displaced from those of a basis structure with space group symmetry (an ordinary crystal). The displacements are given by the *atomic modulation function* $\mathbf{u}_{\mathrm{j}}(\mathbf{r})$, where *j* indicates the *j*th atom in the unit cell of the basic structure.

$$r(n,j) \;=\; n+r_j+u_j(n+r_j).$$

The modulation function has a Fourier expansion

$$u_j(r) \;=\; \textstyle\sum_k \hat{u}(k)\exp(2\pi ik.\,r),\; with\; k=\sum_{i=1}^{n} h_i a_i^*,$$

with finite value of *n*. If *n*=1, the modulated structure is one-dimensionally modulated. A special case of a one-dimensionally modulated structure is

$$r(n,j)_\alpha \;=\; n_\alpha+r_{j\alpha}+A_{j\alpha}\sin(2\pi iq.\,n+r_j)+\phi_{j\alpha}),\,(\alpha=x,y,z).$$

1.36: Domain of influence

The domain of influence of a lattice point *P* (Delaunay 1933), or Dirichlet domain or Voronoi domain, consists of all points *Q* in space that are closer to this lattice point than to any other lattice point or at most equidistant to it, namely such that **OP** ≤|**t** - **OP**| for any vector **t** belonging to the vector lattice *L*. It is the inside of the Wigner-Seitz cell.

1.37: Double coset

Let G be a group, and H and K be two subgroups of G. One says that the two elements $g_1 \in G$ and $g_2 \in G$ belong to the same **double coset** of G relative to H and K if there exist elements $h_i \in H$ and $k_j \in K$ such that:

$g_2 = h_i g_1 k_j$

The complex Hg_1K is called a **double coset**

The partition of G into double cosets relative to H and K is a classification, *i.e*. each $g_i \in G$ belongs to exactly one double coset. It is also a generalization of the coset decomposition, because the double coset Hg_1K contains complete left cosets of K and complete right cosets of H.

1.38: Dual basis

1.39: D centered cell

The **D centered cell** is the used for the rhombohedral description of the hexagonal lattice. Six right-handed *D* cell with basis vectors of equal length are obtained from the *hP* cell by means of one of the following transformation matrices:

D_1: 10-1/01-1/111 D_2: -101/0-11/111

the other four *D* cells are obtained by cyclic permutation of the basis vectors.

The resulting *hD* cell has centering nodes at 1/3,1/3,1/3 and 2/3,2/3,2/3

1.40: Eigensymmetry

The *eigensymmetry*, or *inherent symmetry*, of a crystal is the point group or space group of a crystal, irrespective of its orientation and location in space. For instance, all individuals of a twinned crystal have the same (or the enantiomorphic) eigensymmetry but may exhibit different orientations. The orientations of each of two twin components are related by a twin operation which cannot be part of the eigensymmetry.

In morphology, the eigensymmetry is the full symmetry of a crystalline form, considered as a polyhedron by itself. The eigensymmetry point group is either the generating point group itself or a supergroup of it.

1.41: Euclidean mapping

The **Euclidean mapping** or **isometry** is a special case of affine mapping that, besides collinearity and ratios of distances, keeps also *distances* and *angles*. Because of this, a Euclidean mapping is also called a *rigid motion*.

Euclidean mappings are of three types:

- translations
- rotations
- reflections.

A special case of Euclidean mapping is a symmetry operation.

1.42: Factor group

Let N be a normal subgroup of a group G. The **factor group** or **quotient group** G/N is the set of all left cosets of N in G, i.e.:

$$G/N = \{aN : a\backslash\text{isin}G\}.$$

For each aN and bN in G/N, the product of aN and bN is (aN)(bN), which is still a left coset. In fact, because N is normal:

$$(aN)(bN) = a(Nb)N = a(bN)N = (ab)NN = (ab)N.$$

The inverse of an element aN of G/N is $a^{-1}N$.

1.43: Family structure

By superposing two or more identical copies of the same polytype translated by a superposition vector (*i.e.* a vector corresponding to a submultiple of a translation period) a fictitious structure is obtained, which is termed a *superposition structure*. Among the infinitely possible superposition structures, that structure having all the possible positions of each OD layers is termed a **family structure**: it exists only if the shifts between adjacent layers are rational, i.e. if they correspond to a submultiple of lattice translations.

The family structure is common to all polytypes of the same family. From a group-theoretical viewpoint, building the family structure corresponds to transforming ("completing") all the local symmetry operations of a space groupoid into the global symmetry operations of a space-group.

1.44: Fixed-point-free space groups

Space groups with no special Wyckoff positions (*i.e.* with no special crystallographic orbits) are called **fixed-point-free space groups** or **torsion-free space groups** or **Bieberbach groups**. In fixed-point-free space groups group every element other than the identity has infinite order.

1.45: Flack parameter

The Flack parameter is the molar fraction x in the defining equation $C=(1-x)X+x\bar{X}$, where C represents an oriented two-domain-structure crystal, twinned by inversion, consisting of an oriented domain structure X and an oriented inverted domain structure $\bar{X}$. In reciprocal space, the Flack parameter x is defined by the structure-amplitude equation

$$G^2(h,k,l,x)=(1-x)|F(h,k,l)|^2+x|F(\bar{h},\bar{k},\bar{l}\,)|^2 .$$

For a multidomain-structure twin of a chiral crystal structure, an equivalent Flack parameter may be calculated according to the method of Flack and Bernardinelli (1999).

1.46: Form

For a point group P a **form** is a set of all symmetrically equivalent "elements", namely:

- in vector space, a ***crystal form*** or ***face form*** is a set of all symmetrically equivalent faces;
- in point space, a ***point form*** is a set of all symmetrically equivalent points.

The polyhedron or polygon of a point form is dual to the polyhedron of the corresponding face form, where "dual" means that they have the same number of edges but the number of faces and vertices is interchanged. The inherent symmetry of a form is a point group C which either coincides with the generating point group P or is a supergroup of it.

Forms in point groups correspond to crystallographic orbits in space groups.

1.47: Friedel's law

Friedel's law, or rule, states that the intensities of the h, k, l and $\bar{h}, \bar{k}, \bar{l}$ reflections are equal. This is true either if the crystal is centrosymmetric or if no resonant scattering is present. It is in that case not possible to tell by diffraction whether an inversion center is present or not. The apparent symmetry of the crystal is then one of the eleven Laue classes.

The reason for Friedel's rule is that the diffracted intensity is proportional to the square of the modulus of the structure factor, $|F_h|^2$, according to the geometrical, or kinematical theory of diffraction. It depends similarly on the modulus of the structure factor according to the dynamical theory of diffraction. The structure factor is given by:

$$F_h = \Sigma_j f_j \exp - 2\pi \mathrm{i} \backslash \mathrm{bold} h. \backslash \mathrm{bold} r_j$$

where f_j is the atomic scattering factor of atom j, **h** the reflection vector and $\backslash \mathrm{bold} r_j$ the position vector of atom j. There comes:

$$|F_h|^2 = F_h F_{\bar{h}}^* = F_h F_{\bar{h}} = |F_{\bar{h}}|^2$$

if the atomic scattering factor, f_j, is real. The intensities of the h, k, l and $\bar{h}, \bar{k}, \bar{l}$ reflections are then equal. If the crystal is absorbing, however, due to resonant scattering, the atomic scattering factor is complex and

$$F_{\bar{h}} \neq F_h^*$$

The reflections h, k, l and $\bar{h}, \bar{k}, \bar{l}$ are called a Friedel pair. They are used in the resolution of the phase problem for the solution of crystal structures and in the determination of absolute structure.

History

Friedel's law was stated by G. Friedel (1865-1933) in 1913 (Friedel G., 1913, *Sur les symétries cristallines que peut révéler la diffraction des rayons X.*, *C.R. Acad. Sci. Paris*, **157**, 1533-1536.

See also

Absolute structure
Section 3.1 of *International Tables of crystallography, Volume A*

1.48: Geometric crystal class

Geometric crystal classes (or simply 'crystal classes') classify the symmetry groups of the external shape of macroscopic crystals, namely according to the morphological symmetry. There are 10 two-dimensional geometric crystal classes and 32 three-dimensional geometric crystal classes, in one to one correspondence with the 10 and 32 types of point groups in E^2 and E^3, respectively.

See also

- Section 8.2.4 of *International Tables for Crystallography, Volume A*

Contributors

1.49: Geometric element

A **geometric element** is an element in space (plane, line, point, or a combination of these) about which asymmetry operation is performed. Geometric elements are classified on the basis of the dimensionality N of the space on which they act, the upper limit on the dimensionality of the symmetry element being N-1.

1.50: Group

A set G equipped with a binary operation $*$: $G \times G \to G$, assigning to a pair (g,h) the product $g*h$ is called a **group** if:

1. The operation is *associative*, i.e. $(a*b)*c = a*(b*c)$.
2. G contains an *identity element* (*neutral element*) e: $g*e = e*g = g$ for all g in G
3. Every g in G has an *inverse element* h for which $g*h = h*g = e$. The inverse element of g is written asg^{-1}.

Often, the symbol for the binary operation is omitted, the product of the elements g and h is then denoted by the concatenation gh.

The binary operation need not be commutative, i.e. in general one will have $g*h \neq h*g$. In the case that $g*h = h*g$ holds for all g,h in G, the group is an Abelian group.

A group G may have a finite or infinite number of elements. In the first case, the number of elements of G is the **order** of G, in the latter case, G is called an **infinite group**. Examples of infinite groups are space groups and their translation subgroups, whereas point groups are finite groups.

1.51: Groupoid

A **groupoid** (G,*) is a set G with a law of composition * mapping of a subset of G x G into G. The properties of a groupoid are:

- if x, y, z ∈ G and if one of the compositions (x*y)*z or x*(y*z) is defined, so is the other and they are equal; (associativity);
- if x, x' and y ∈ G are such that x*y and x'*y are defined and equal, then x = x'; (cancellation property)
- for all x ∈ G there exist elements e_x (left unit of x), e_x' (right unit of x) and x^{-1} ("inverse" of x) such that:
  - $e_x*x = x$
  - $x* e_x' = x$
  - $x^{-1}*x = e_x'$.

From these properties it follows that:

- $x* x^{-1} = e_x$, *i.e.* that that e_x is right unit for x^{-1},
- e_x' is left unit for x^{-1}
- e_x and e_x' are idempotents, *i.e.* $e_x* e_x = e_x$ and $e_x'* e_x' = e_x'$.

The concept of groupoid as defined here was introduced by Brandt (1927). An alternative meaning of groupoid was introduced by Hausmann & Ore (1937) as a set on which binary operations act but neither the identity nor the inversion are included. For this second meaning nowadays the term **magma** is used instead (Bourbaki, 1998).

1.52: Group homomorphism

1.53: Group isomorphism

A **group isomorphism** is a special type of group homomorphism. It is a mapping between two groups that sets up a one-to-one correspondence between the elements of the groups in a way that respects the respective group operations. If there exists an isomorphism between two groups, then the groups are called **isomorphic**. Isomorphic groups have the same properties and the same structure of their multiplication table.

Let $(G, *)$ and $(H, \#)$ be two groups, where "*" and "#" are the binary operations in G and H, respectively. A *group isomorphism* from $(G, *)$ to $(H, \#)$ is a bijection from G to H, *i.e.* a bijective mapping $f : G \to H$ such that for all u and v in G one has

$$f(u * v) = f(u) \# f(v).$$

Two groups $(G, *)$ and $(H, \#)$ are isomorphic if an isomorphism between them exists. This is written:

$$(G, *) \cong (H, \#)$$

If $H = G$ and the binary operations # and * coincide, the bijection is an automorphism.

1.54: Hemihedry

The point group of a crystal is called hemihedry if it is a subgroup of index 2 of the point group of its lattice.

1.55: Holohedry

The point group of a crystal is called holohedry if it is identical to the point group of its lattice. In the three-dimensional space, there are seven holohedral geometric crystal classes: $\bar{1}, 2/m, mmm, \bar{3}m, 4/mmm, 6/mmm, m\bar{3}m$

1.56: H centered cell

The **H centered cell** (**triple hexagonal cell**) is an alternative description of the hexagonal Bravais lattice. From the conventional *hP* cell one obtains the *hH* cell by taking the new basis vectors by means of one of the following transformation matrices, which give three possible orientations of the *hH* cell with respect to the *hP* cell:

$$H_1\text{: 110/-120/001 } H_2\text{: 2-10/110/001 } H_3\text{: 1-20/2-10/001}$$

The resulting *hH* cell has centering nodes at 1/3,2/3,0 and 2/3,1/3,0.

Secondary and tertiary elements in the *hP* cell are exchanged in the *hH* cell. For example, the space-group symbol $P3m1$ become $H31m$ when the triple cell is used.

1.57: Image

Let X and Y be sets, f be the function $f : X \to Y$, and x be some member of X. Then the **image** of x under f, denoted $f(x)$, is the unique member y of Y that f associates with x.

The **image** of a subset $A \subseteq X$ under f is the subset of Y defined by $f[A] = \{y \in Y \mid y = f(x) \text{ for some } x \in A\}$.

1.58: Incommensurate composite crystal

An *incommensurate composite crystal* is a compound with two or more (*N*) subsystems that are themselves modulated structures, with basis structures that are mutually incommensurate. Each subsystem (numbered by ν) has a reciprocal lattice for its basic structure with three basis vectors $a_i^{*\nu}$. There is a basis of the vector module of diffraction spots that has at most 3*N* basis vectors A_j^* such that

$$a_i^{*\nu} = \sum_{j=1}^{n} Z_{ij}^{\nu} A_j^* \quad (i = 1, 2, 3),$$

where Z_{ij}^{ν} are integer coefficients. If *n* is larger than the dimension of space (three), the composite crystal is an aperiodic crystal. *n* is the rank of the vector module.

1.59: Incommensurate magnetic structure

An *incommensurate magnetic structure* is a structure in which the magnetic moments are ordered, but without periodicity that is commensurate with that of the nuclear structure of the crystal. In particular, the magnetic moments have a spin density with wave vectors that have at least one irrational component with respect to the reciprocal lattice of the atoms. Or, in the case of localized moments, the spin function $\mathbf{S}(\mathbf{n}+\mathbf{r}_j)$ (where the jth atom has position $\mathbf{r}_j$ in the unit cell) has Fourier components with irrational indices with respect to the reciprocal lattice of the crystal.

1.60: Incommensurate modulated structure

An *incommensurate modulated crystal structure* is a modulated crystal structure, for which the modulation function has a Fourier transform of sharp peaks at wave vectors that cannot all be expressed by rational coefficients in a basis of the reciprocal lattice of the basic structure. At least one of the components of the wave vectors of the modulation with respect to the basis structure should be irrational.

Contributors

1.61: Lattice

A **lattice** in the vector space $\mathbf{V^n}$ is the set of all integral linear combinations $\mathbf{t} = u_1\mathbf{a_1} + u_2\mathbf{a_2} + \ldots + u_k\mathbf{a_k}$ of a system ($\mathbf{a_1}$, $\mathbf{a_2}$, ... , $\mathbf{a_k}$) of linearly independent vectors in $\mathbf{V^n}$.

If $k = n$, i.e. if the linearly independent system is a **basis** of $\mathbf{V^n}$, the lattice is often called a **full lattice**. In crystallography, lattices are almost always full lattices, therefore the attribute "full" is usually suppressed.

1.62: Lattice complex

A *lattice complex* is the set of all point configurations that may be generated within one type of Wyckoff set. All Wyckoff positions, Wyckoff sets and types of Wyckoff sets that generate the same set of point configurations are assigned to the same lattice complex.

Concretely, two Wyckoff positions are assigned to the same lattice complex if there is a suitable transformation that maps the point configurations of the two Wyckoff positions onto each other and if their space groups belong to the same crystal family. The 72 (in E^2) or 1731 (in E^3) Wyckoff positions are classified in 51 (E^2) or 1128 (E^3) types of Wyckoff sets. They are assigned to 30 (E^2) or 402 (E^3) lattice complexes.

The name *lattice complex* comes from the fact that an assemblage of points that are equivalent with respect to a group of symmetry operations including lattice translations can be visualized as a set of equivalent lattices.

1.63: Lattice system

A **lattice system** of space groups contains complete Bravais flocks. All those Bravais flocks which intersect exactly the same set of geometric crystal classes belong to the same lattice system.

All those Bravais flocks belong to the same lattice system for which the Bravais classes belong to the same (holohedral) geometric crystal class.

1.64: Laue classes

The Laue classes correspond to the eleven centrosymmetric crystallographic point groups. When absorption is negligible and Friedel's law applies, it is impossible to distinguish by diffraction between a centrosymmetric point group and one of its non-centrosymmetric subgroups.

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Laue classes	Non-centrosymmetric groups having the same Laue class
$\bar{1}$	1
$2/m$	2, m
mmm	222, $2mm$
$\bar{3}$	3
$\bar{3}m$	32, $3m$
$4/m$	4, $\bar{4}$
$4/mmm$	422, $\bar{4}2m$, $42m$
$6/m$	6, $\bar{6}$
$6/mmm$	622, $\bar{6}2m$, $62m$
$m\bar{3}$	23
$m\bar{3}m$	432, $\bar{4}32$

1.65: Limiting complex

A **limiting complex** is a lattice complex L1 which forms a true subset of a second lattice complex L2. Each point configuration of L1 also belongs to L2.

L2 is called a **comprehensive complex** of L1.

1.66: Local symmetry

A motion of E^n mapping onto itself a subdomain of a crystal pattern but not the whole crystal pattern is called a **local symmetry operation**. It may be crystallographic or noncrystallographic depending on whether or not it is possible to extend the subdomain to an *n*-dimensional crystal pattern invariant under the motion.

Contributors

1.67: Mapping

The term **mapping** is often used in mathematics as a synonym of *function*. In crystallography it is particularly used to indicate a *transformation*.

1.68: Merohedral

Merohedral is the adjectival form of merohedry and indicates a crystal that does not possess the full point symmetry of its lattice.

1.69: Merohedry

The point group of a crystal is called merohedry if it is a subgroup of the point group of its lattice.

1.70: Mesh

In a two-dimensional pattern possessing rotational symmetry, the rotation points constitute the nodes of a net and divide the plane into regions that are called **meshes**. The number of meshes meeting at any rotation point equals twice the order of the rotation at that point.

N.B. The term **mesh** is sometimes *improperly* used to indicate a two-dimensional cell.

1.71: Miller Indices

1.72: Modulated crystal structure

A *modulated crystal structure* is a density (or atom arrangement) that may be obtained from a density (or atom arrangement) with space-group symmetry by a finite density change (or finite displacement of each atom, respectively) that is (quasi)periodic. A function or a displacement field is periodic if it is invariant under a lattice of translations. Then its Fourier transform consists of δ-peaks on a reciprocal lattice that spans the space and is nowhere dense. A quasiperiodic function has a Fourier transform consisting of δ-peaks on a vector module of finite rank. This means that the peaks may be indexed with integers using a finite number of basis vectors . If the modulation consists of deviations from the basic structure in the positions, the modulation is *displacive* (displacive modulation). When the probability distribution deviates from that in the basic structure the modulation is occupational.

See also

Model for a displacively modulated crystal structure . The basic structure is two-dimensional rectangular, with lattice constants *a* and *b*, the modulation wave vector is in the *b*-direction, the wavelength of the periodic modulation is λ such that λ/*b* is an irrational number.

Contributors

1.73: Normalizer

Given a group G and one of its supergroups S, they are uniquely related to a third, intermediated group $N_S(G)$, called the **normalizer of G with respect to S**. $N_S(G)$ is defined as the set of all elements **S** ∈ S that map G onto itself by conjugation:

$$N_S(G) := \{\mathbf{S} \in S \mid \mathbf{S}^{-1}G\mathbf{S} = G\}$$

The normalizer $N_S(G)$ may coincide either with G or with S or it may be a proper intermediate group. In any case, G is a normal subgroup of its normalizer.

1.74: Normal subgroup

A subgroup H of a group G is **normal** in G ($H \triangleleft G$) if $gH = Hg$ for any $g \in G$. Equivalently, $H \subset G$ is normal if and only if $gHg^{-1} = H$ for any $g \in G$, i.e., if and only if each conjugacy class of G is either entirely inside H or entirely outside H. This is equivalent to say that H is invariant under all inner automorphisms of G.

The property $gH = Hg$ means that left and rights cosets of H in G coincide. From this one sees that the cosets form a group with the operation $g_1H * g_2H = g_1g_2H$ which is called the factor group or **quotient group** of G by H, denoted by G/H.

In the special case that a subgroup H has only two cosets in G (namely H and gH for some g not contained in H), the subgroup H is always normal in G.

1.75: OD structure

OD structures consist of slabs with their own symmetry, containing coincidence operations constituting a diperiodic group(layer group) only within individual slabs. For the entire structure these coincidence operations are only local (partial), i.e. they are valid only in a subspace of the crystal space. The ambiguity (= existence of more than one equivalent possibilities) in the stacking of slabs arises from the existence of this local symmetry, which does not appear in the space group of the structure. The resulting structure can be "ordered" (*periodic*) or "disordered" (*non-periodic*), depending on the sequence of local symmetry operations relating pairs of slabs. The set of all the operations valid in the whole crystal space constitutes a space group; by adding the set of all the operations valid in a subspace of it, one obtains a space groupoid.

In the OD theory, a central role is played by the **vicinity condition** (**VC**), which states the geometrical equivalence of layer pairs. The vicinity condition consists of three parts:

- **VC α**: VC layers are either geometrically equivalent or, if not, they are relatively few in kind
- **VC β**: translation groups of all VC layers are either identical or they have a common subgroup
- **VC γ**: equivalent sides of equivalent layers are faced by equivalent sides of adjacent layers so that the resulting pairs are equivalent.

If the position of a layer is uniquely defined by the position of the adjacent layers and by the VC, the resulting structure is fully ordered. If, on the other hand, more than one position is possible that obeys the VC, the resulting structure is an **OD structure** and the layers are **OD layers**. VC structures may thus be either fully ordered structures or OD structures. All OD structures are polytypic; the reverse may or may not be true. Equivalency depends on the choice of OD layers and also on the definition of polytypism.

1.76: Ogdohedry

The point group of a crystal is called ogdohedry if it is a subgroup of index 8 of the point group of its lattice.

In the three dimensional space there is only one ogdohedry: it corresponds to the geometric crystal class 3 of crystals belonging to the hexagonal lattice system (in case rhombohedral crystals, it corresponds instead to a tetartohedry).

1.77: Order

If G is a group consisting of a finite number of elements, this number of elements is the **order** of G. For example, the point group `m3m` has order 48.

For an element g of a (not necessarily finite) group G, the **order** of g is the smallest integer n such that g^n is the identity element of G. If no such integer exists, g is of **infinite order**. For example, the rotoinversion `3` has order 6 and a translation has infinite order. An element of order 2 is called an **involution**.

1.78: Partial symmetry

The symmetry operations of a space group are isometries operating on the whole crystal pattern and are also called **total operations** or **global operations**. More generally, the crystal space can be divided in N components S_1 to S_N, and a coincidence operation $\varphi(S_i) \to S_j$ can act on just the i-th component S_i to bring it to coincide with the j-th component S_j. Such an operation is not one of the operations of the space group of the crystal because it is not a coincidence operation of the whole crystal space; it is not even defined, in general, for any component k different from i. It is called a **partial operation**: from the mathematical viewpoint, partial operations are space-groupoid operations.

When $i = j$, *i.e*. when the operation is $\varphi(S_i) \to S_i$ and brings a component to coincide with itself, the partial operation is of special type and is called **local**. A local operation is in fact a symmetry operation, which is defined only on a part of the crystal space: local operations may constitute a subperiodic group.

1.79: Patterson methods

The family of methods employed in structure determination to derive relationships between the scattering centers in a crystal lattice when the diffraction phases are unknown. They depend upon interpretation of the *Patterson function*

$$P(uvw) = \frac{1}{V} \sum_h \sum_k \sum_l |F(hkl)|^2 \cos[2\pi(hu + kv + lw)]$$

to reveal interatomic vectors within the unit cell.

1.80: Patterson vector

A real-space vector representing the difference between two position vectors locating scattering centers in a diffracting crystal lattice .

1.81: Point configuration

The concept of *point configuration* is closely related to that of crystallographic orbit, but differs from it by the fact that point configurations are detached from their generating space groups. The concept of point configuration is the basis for the definition of lattice complexes.

Two crystallographic orbits are said *configuration-equivalent* if and only if their sets of points are identical. A **point configuration** is the set of all points that is common to a class of configuration-equivalent crystallographic orbits.

This definition uniquely assigns crystallographic orbits to point configurations but not *vice versa*.

The *inherent* symmetry of a point configuration is the most comprehensive space group that maps the point configuration onto itself. One crystallographic orbit out of each class of configuration-equivalent ones stands out because its generating space group coincides with the inherent symmetry of its point configuration.

1.82: Point group

A **point group** is a group of symmetry operations all of which leave at least one point unmoved. A *crystallographic* point group is a point group that maps a point lattice onto itself: in three dimensions rotations and rotoinversions are restricted to 1, 2, 3, 4, 6 and $\bar{1}$, $\bar{2}$ (= *m*), $\bar{3}$, $\bar{4}$, $\bar{6}$ respectively.

1.83: Point space

A mathematical model of the space in which we live is the **point space**. Its elements are points. Objects in point space may be single points; finite sets of points like the centers of the atoms of a molecule; infinite discontinuous point sets like the centers of the atoms of an ideal crystal pattern; continuous point sets like straight lines, curves, planes, curved surfaces, etc.

Objects in point space are described by means of a coordinate system referred to point chosen as the origin O. An arbitrary point P is then described by its coordinates x, y, z.

The point space used in crystallography is a Euclidean space, *i.e.* an affine space where the scalar product is defined.

Crystal structures are described in point space. The vector space is a dual of the point space because to each pair of points in point space a vector in vector space can be associated.

1.84: Point symmetry

The point symmetry of a position is its site symmetry. The point symmetry, or point group of a lattice is the group of linear mappings (symmetry operations, isometries) that map the vector lattice **L** onto itself. Those geometric crystal classes to which point symmetries of lattices belong are called holohedries.

1.85: Polytypism

An element or compound is **polytypic** if it occurs in several structural modifications, each of which can be regarded as built up by stacking layers of (nearly) identical structure and composition, and if the modifications differ only in their stacking sequence. Polytypism is a special case of polymorphism: the two-dimensional translations within the layers are essentially preserved.

The complete definition is given in the Report of the International Union of Crystallography Ad-Hoc Committee on the Nomenclature of Disordered, Modulated and Polytype Structures: *Acta Cryst.* A**40**, 399-404(1984), "Nomenclature of Polytype Structures".

1.86: Primitive basis

A primitive basis is a crystallographic basis of the vector lattice **L** such that every lattice vector **t** of **L** may be obtained as an integral linear combination of the basis vectors, **a**, **b**, **c**.

In mathematics, a primitive basis is often called a *lattice basis*, whereas in crystallography the latter has a more general meaning and corresponds to a crystallographic basis.

1.87: Primitive cell

A primitive cell is a unit cell built on the basis vectors of a primitive basis of the direct lattice, namely a crystallographic basis of the vector lattice **L** such that every lattice vector **t** of **L** may be obtained as an integral linear combination of the basis vectors, **a**, **b**, **c**.

It contains only one lattice point and its volume is equal to the triple scalar product (**a**, **b**, **c**).

Non-primitive bases are used conventionally to describe *centered lattices*. In that case, the unit cell is a multiple cell and it contains more than one lattice point. The multiplicity of the cell is given by the ratio of its volume to the volume of a primitive cell.

1.88: Priority rule

When more than one kind of symmetry element occurs for a given symmetry direction, the choice for defining the appropriate Hermann–Mauguin symbol for the space group is made in order of descending priority:

- *m*, *e*, *a*, *b*, *c*, *n*, *d*;
- rotation axes before screw axes.

There are a few exceptions to this choice:

1. For glide planes in centered monoclinic space groups, the priority rule is purposely not followed in order to bring out the relations between the three ‘cell choices’ given for each setting.
2. For orthorhombic space groups, the priority rule is applied only to the ‘standard symbol’. The symbols for the other five settings are obtained from the standard symbol by the appropriate transformations, without invoking the priority rule again.
3. Space-group types $I222$ and $I2_12_12_1$ are two distinct types. Both contain parallel twofold rotation and screw axes and thus would receive the same symbol according to the priority rule. In $I222$, the three rotation axes and the three screw axes intersect, whereas in $I2_12_12_1$ neither the three rotation axes nor the three screw axes intersect.
4. For space groups of type No. 73, the standard symbol *Ibca* was adopted, instead of *Ibaa* according to the rule, because Ibca displays the equivalence of the three symmetry directions clearly.
5. In tetragonal space groups with both *a* and *b* glide planes containing the [001] direction, the preference was given to *b*, as in *P4bm*.
6. In cubic space groups where tertiary symmetry planes with glide components 1/2, 0, 0; 0, 1/2, 0; 0, 0, 1/2 and 1/2, 1/2 , 1/2 coexist, the tertiary symmetry element was called *n* in *P* groups (instead of *a*, *b* or *c*) but *c* in *F* groups, because these symmetry elements intersect the origin.
7. Space groups of type $I23$ and $I2_13$ (199) are two distinct types of space groups. For this pair, the same arguments apply as given above for $I222$ and $I2_12_12_1$.

1.89: Pseudo symmetry

A crystal space can in general be divided in N components S_1 to S_N. When a coincidence operation $\varphi(S_i) \rightarrow S_j$ brings the i-th component S_i to coincide with the j-th component S_j, for any i and j, φ is a symmetry operation of the space group.

Sometimes, φ brings S_i close to, but not exactly on, the position and orientation of S_j: in this case the operation mapping S_i onto S_j is not crystallographic but the linear and/or rotational deviation from a space group operation is limited. For this reason, it is preferable to describe the crystallographic operation φ as a **pseudo symmetry operation**.

Pseudo symmetry operations for the lattice play an important role in twinning, namely in the case of twinning by pseudomerohedry and twinning by reticular pseudomerohedry.

1.90: Reciprocal lattice

The reciprocal lattice is constituted by the set of all possible linear combinations of the basis vectors $\mathbf{a^*}$, $\mathbf{b^*}$, $\mathbf{c^*}$ of the reciprocal space. A point (*node*), H, of the reciprocal lattice is defined by its position vector:

$$\mathbf{OH} = \mathbf{r_{hkl}}^* = h\,\mathbf{a^*} + k\,\mathbf{b^*} + l\,\mathbf{c^*}.$$

If H is the nth node on the row OH, one has:

$$\mathbf{OH} = n\,\mathbf{OH_1} = n\,(h_1\,\mathbf{a^*} + k_1\,\mathbf{b^*} + l_1\,\mathbf{c^*}),$$

where H_1 is the first node on the row OH and h_1 , k_1 , l_1 are relatively prime.

The generalization of the reciprocal lattice in a four-dimensional space for incommensurate structures is described in Section 9.8 of *International Tables of Crystallography, Volume C*.

1.91: Reciprocal Space

The basis vectors **a***, **b***, **c*** of the reciprocal space are related to the basis vectors **a**, **b**, **c** of the direct space (or crystal space) through either of the following two equivalent sets of relations:

(1)

a*. **a** = 1; **b***. **b** = 1; **c***. **c** = 1;

a*. **b** = 0; **a***. **c** = 0; **b***. **a** = 0; **b***. **c** = 0; **c***. **a** = 0; **c***. **b** = 0.

(2)

a* = (**b** × **c**)/ (**a**, **b**, **c**);

b* = (**c** × **a**)/ (**a**, **b**, **c**);

c* = (**b** × **c**)/ (**a**, **b**, **c**);

where (**b** × **c**) is the vector product of basis vectors **b** and **c** and (**a**, **b**, **c**) = *V* is the triple scalar product of basis vectors **a**, **b**and **c** and is equal to the volume *V* of the cell constructed on the vectors **a**, **b** and **c**.

The reciprocal and direct spaces are reciprocal of one another, that is the reciprocal space associated to the reciprocal space is the direct space. They are related by a Fourier transform and the reciprocal space is also called *Fourier space* or *phase space*.

The **vector product** of two direct space vectors, $\backslash\text{bold}r_1 = u_1\backslash\text{bold}a + v_1\backslash\text{bold}b + w_1\backslash\text{bold}c$ and $\backslash\text{bold}r_2 = u_2\backslash\text{bold}a + v_2\backslash\text{bold}b + w_2\backslash\text{bold}c$ is a reciprocal space vector,

{\bold r*} = {\bold r_1} \times {\bold r_2} = V (v_1 w_2 - v_2 w_1) {\bold a*} + V (w_1 u_2 - w_2 u_1) {\bold b*} + V (u_1 v_2 - u_2 v_1) {\bold c}.

Reciprocally, the vector product of two reciprocal vectors is a direct space vector.

As a consequence of the set of definitions (1), the **scalar product** of a direct space vector **r** = *u* **a** + *v* **b** + *w* **c** by a reciprocal space vector **r*** = *h* **a*** + *k* **b*** + *l* **c*** is simply:

r . **r*** = *uh* + *vk* +*wl*.

In a **change of coordinate system**, The coordinates of a vector in reciprocal space transform like the basis vectors in direct space and are called for that reason *covariant*. The vectors in reciprocal transform like the coordinates in direct space and are called *contravariant*.

1.92: Semidirect product

In group theory, a **semidirect product** describes a particular way in which a group can be put together from two subgroups, one of which is normal.

Let G be a group, N a normal subgroup of G (i.e., $N \lhd G$) and H a subgroup of G. G is a **semidirect product** of N and H if there exists a homomorphism $G \rightarrow H$ which is the identity on H and whose kernel is N. This is equivalent to say that:

- $G = NH$ and $N \cap H = \{1\}$ (where "1" is identity element of G)
- $G = HN$ and $N \cap H = \{1\}$
- Every element of G can be written as a unique product of an element of N and an element of H
- Every element of G can be written as a unique product of an element of H and an element of N

One also says that "G *splits* over N".

1.93: Site symmetry

The site-symmetry group (often called point symmetry) of a point is the finite group formed by the set of all symmetry operations of the space group of the crystal that leave that point invariant. It is isomorphic to a (proper or improper)subgroup of the point group to which the space group under consideration belongs. In general, the origin is a point of highest site symmetry.

1.94: Space group

The symmetry group of a three-dimensional crystal pattern is called its **space group**. In E^2, the symmetry group of a two-dimensional crystal pattern is called its **plane group**. In E^1, the symmetry group of a one-dimensional crystal pattern is called its **line group**.

To each crystal pattern belongs an infinite set of translations **T**, which are symmetry operations of that pattern. The set of all **T** forms a group known as the **translation subgroup** T of the space group G of the crystal pattern. T is an Abelian group.

1.95: Stabilizer

Let G be a group which acts on a set A by a composition law *, and let a be a given element of A. Then the set: G_a = {g ∈ G | a*g = a} is called the **stabilizer** of A. G_a is the set of all elements of G which leave a unchanged or 'stable'. G_a is a subgroup of G.

1.96: Statistical descriptors

A separate online document Statistical Descriptors in Crystallography prepared for the International Union of Crystallography provides an authoritative statement on some aspects of the use of statistics and statistical techniques in crystallography, principally that of least-squares refinement of diffraction data against an atomic model. The following topics are treated:

- Glossary
- Basic notions
- Uncertainty of measurement
- Refinement
- Refinement on I, $|F|^2$ or $|F|$?
- Defects in the model
- Weighting schemes
- **Recommendations**

1.97: Subcell

A cell C' obtained from a cell C by adding one or more translation vectors of fractional periodicity in C is called a **subcell** of C. The translation subgroup **T'** of the lattice **L'** built on C' is a supergroup of the translation subgroup **T** of the lattice **L** built on C and corresponds therefore to superlattice of **L**.

1.98: Subgroup

Let G be a group and H a non-empty subset of G. Then H is called a **subgroup** of G if the elements of H obey the group postulates, i.e. if

1. the identity element 1_G of G is contained in H;
2. H is closed under the group operation (inherited from G);
3. H is closed under taking inverses.

The subgroup H is called a **proper subgroup** of G if there are elements of G not contained in H.

A subgroup H of G is called a **maximal subgroup** of G if there is no proper subgroup M of G such that H is a proper subgroup of M.

1.99: Sublattice

A lattice **L'** obtained by another lattice **L** by removing one or more sets of nodes is called a **sublattice of L**. The translation subgroup **T'** of **L'** is a subgroup of the translation subgroup **T** of **L**. The unit cell of **L'** is larger than the unit cell of **L** and is therefore called a supercell.

Contributors

CHAPTER OVERVIEW

2: History of Crystallography

Crystallography (from the Greek words crystallon = cold drop / frozen drop, with its meaning extending to all solids with some degree of transparency, and graphein = write) is the experimental science of determining the arrangement of atoms in solids. In older usage, it is the scientific study of crystals.

Topic hierarchy

2.1: Lepton

Lepton is a term introduced by Friedrich Rinne in his book *Crystals and the Fine-Structure of Matter*(London: Methuen & Co., 1924, English translation by S. W. Stiles) to indicate electrons, atoms, ions, radicals, and molecules building the unit formula of a crystalline compound. The crystal structure of a solid was sometimes called "leptonic structure".

Today, the term lepton is used to indicate spin-1/2 particles and Rinne's use is only of historical interest.

CHAPTER OVERVIEW

3: X-rays

Topic hierarchy

3.1: Absorption edge

An absorption edge is a sharp discontinuity in the absorption spectrum of X-rays by an element that occurs when the energy of the photon corresponds to the energy of a shell of the atom (K, L_I, L_{II}, L_{III}, etc.).

3.2: Anomalous absorption

Anomalous absorption takes place when radiation is dynamically diffracted by a perfect or nearly perfect crystal. The optical field in the crystal is then made up by several components, called wavefields, two in the two beam case (neglecting polarization in the X-ray case). One of them is absorbed more than normal and the other one less than normal. In the transmission, or Laue geometry, both wavefields propagate inside the crystal; one then speaks of anomalous transmission for the less absorbed wavefield (Borrmann effect). In the reflection, or Bragg geometry, one wavefield only propagates in the crystal, the more absorbed one for angles of incidence corresponding to one side of the total reflection rocking curve and the less absorbed one for the other side. This results in an asymmetry of the rocking curve that is calculated using dynamical theory.

3.3: Anomalous dispersion

The 'anomalous' dispersion corrections, which are not in fact anomalous, take into account the effect of absorption in the scattering of phonons by electrons. In the classic picture the electron is approximated by a damped harmonic oscillator. The scattering factor of the electron is then complex and the atomic scattering factor, or atomic form factor, is given by:

$f + f' + \mathrm{i} f''$

where f' and f'' are the real and imaginary parts of the anomalous dispersion correction. Their importance increases as one gets closer to an absorption edge (resonant scattering). Numerical calculations usually follow the Hartree-Fock approximations. For details on the non-relativistic and relativistic approaches, see Section 4.2.6 of *International Tables of Crystallography, Volume C*.

3.4: Anomalous scattering

The history of the description of the scattering of an atom when illuminated with X-rays is that initially wavelength dependencies were ignored. This was initially referred to as 'normal scattering'. The wavelength dependencies were then corrections to the normal scattering and also called anomalous. These had to describe changes in amplitude and phase, respectively initially given the symbols $\Delta f'$ and $\Delta f''$. Thus the X-ray scattering factor of an atom is described by the equation:-

$$f = f_o + \Delta f' + i\Delta f''$$

The nomenclature changed when tunable synchrotron sources became available and whereby the Δ prefixes were removed because changes between two wavlengths would then have required a double Δ label, which is cumbersome. Thus the $\Delta f'$ now means the change in f'between two wavelengths. The Δ prefix to f'' is dropped for consistency even though its use is based on its value at a single wavelength.

The values of f' and f'' change most at the absorption edge of the element in question. Thus this resonance effect sometimes leads to the term being refererred to as 'resonant scattering'. However, since the off resonance f'' effect is extensively used in crystal structure determination of the hand of a molecule (its chirality) 'anomalous scattering' is the best *i.e.* most widely embracing term. Another commonly used term is Multiple-wavelength Anomalous Dispersion ('MAD'), which involves measurements made at the resonance condition and at more than one wavelength obviously.

3.5: Borrmann Effect

Due to anomalous absorption, type 1 wavefields propagate in a perfect or nearly perfect crystal with a less than normal absorption. For details and the physical interpretation, see anomalous absorption.

Super-Borrmann effect

It is the enhancement of the Borrmann effect in a three-beam case, *e.g.* when the \(111\) and $\overline{111}$ reflections are simultaneously excited in a silicon or germanium crystal.

History

The Borrmann effect was first discovered in quartz (Borrmann G., 1941, *Über Extinktionsdiagramme der Röntgenstrahlen von Quarz*. *Physik Z.*, **42**, 157-162) and then in calcite crystals (Borrmann G., 1950, *Die Absorption von Röntgenstrahlen in Fall der Interferenz*. *Z. Phys.*, **127**, 297-323), and interpreted by Laue (Laue, M. von, 1949, *Die Absorption der Röntgenstrahlen in Kristallen im Interferenzfall*. *Acta Crystallogr*. **2**, 106-113).

The super-Borrmann effect was first observed by Borrmann G. and Hartwig W. (1965), *Die Absorption der Röntgenstrahlen im Dreistrahlfall der Interferenz*. *Z. Krist.*, **121**, 401-409.

See also

- Section 5.1 of *International Tables of Crystallography, Volume B* for X-rays
- Section 5.2 of *International Tables of Crystallography, Volume B* for electrons
- Section 5.3 of *International Tables of Crystallography, Volume B* for neutrons

3.6: Bragg's law

Bragg's law provides the condition for a plane wave to be diffracted by a family of lattice planes:

$$2d\sin\theta = n\lambda.$$

where d is the **lattice** spacing, θ the angle between the wavevector of the incident plane wave, $\mathbf{k_o}$, and the lattice planes, λ its wave length and n is an integer, the order of the reflection. It is equivalent to the diffraction condition in reciprocal space and to the Laue equations.

Direct derivation of Bragg's law

- **Reflection from the first plane**

The scattered waves will be in phase whatever the distribution of the point scatterers in the first plane if the angle of the reflected wave vector, $\mathbf{k_h}$, is also equal to θ. This is Snell-Descartes' law of reflection.

- **Reflection from the second plane**

Since the phase of the reflected waves is independent of the position of the point scatterer in the plane, the phase difference between the waves reflected by two successive lattice planes is obtained by choosing arbitrarily a scattering point, A, on the first plane and a scattering point,b on the second plane such that AB is normal to the planes. If C and d are the projections of A on the incident and reflected wave vectors passing through B, it is clear from figure 1 that the path difference between the waves reflected at A and B, respectively, is:

$$CB + BD = 2d\sin\theta$$

and that the two waves will be in phase if this path difference is equal to n λ where n is an integer.

- **Reflection from the third, etc., planes**

If Bragg's relation is satisfied for the first two planes, the waves reflected with wave vector $\mathbf{k_h}$ will be in phase fo all the planes of the family.

Order of the reflection

Bragg's law may also be written:

$$2\left(\frac{d}{n}\right)\sin\theta = \lambda.$$

One may then say that a Bragg reflection of order n on a family of lattice planes or order n is equivalent to reflection of order 1 on a family of fictitious, or imaginary, planes of lattice spacing:

$$d_{hkl} = \frac{d}{n}$$

This fictitious family is associated to the reciprocal lattice vector **OH** where $OH = n/d = 1/d_{hkl}$. The indices of the reflection are: hkl. For instance, the dashed blue lines in Figure 1 correspond to the fistitious planes associated to the second order, $n = 2$.

Extinctions, or systematic absences

If there is a glide plane or a screw axis normal to the lattice planes, the spacing of the actual reflecting planes is$d/2$ for a glide plane and ($d\, p/q$) for a q_p screw axis. Bragg's law should then be written:

$2\,(d/2)\sin\theta = n\,\lambda \Rightarrow 2\,d\sin\theta = 2n\,\lambda$

for a glide plane and

$2\,(d\,p/q)\sin\theta = n\,\lambda \Rightarrow 2\,d\sin\theta = (q/p)n\,\lambda$

for a screw axis q_p.

The reflections of odd order for a glide plane and of order different from (q/p)n for a screw axis are then absent. One speaks of extinctions or systematic absences related to the presence of glide or screw components.

As an example, the case of a 2_1 screw axis. Reflections of odd order will be systematically absent.

Influence of deformation

A deformation that leaves a family of lattice planes (*hkl*) undistorted and its lattice spacing *d* unchanged will not affect the Bragg angle of *kkl*reflections, *e.g.* lattice planes parallel to a screw dislocations.

History

A deformation that leaves a family of lattice planes (*hkl*) undistorted and its lattice spacing *d* unchanged will not affect the Bragg angle of *kkl* reflections, *e.g.* lattice planes parallel to a screw dislocations.

3.7: Bragg angle

In Bragg's law describing the condition for a plane wave to be diffracted from a family of lattice planes, the angle θ between the wavevector of the incident plane wave, $\mathbf{k_o}$, and the lattice planes.

Contributors

3.8: Cromer–Mann coefficients

The set of nine coefficients $a_i, b_i, c\ (i = 1, \ldots, 4)$ in a parameterization of the non-dispersive part of the atomic scattering factor for neutral atoms as a function of (sinθ) / λ:

$$f^0(\sin\theta/\lambda) = \sum_{i=1}^{4} a_i \exp[-b_i(\sin\theta/\lambda)^2] + c$$

for $0 < (\sin\theta)/\lambda < 2.0\ \text{Å}^{-1}$.

This expression is convenient for calculation in crystal structure software suites.

3.9: Dynamical diffraction

When a crystal is perfect or nearly perfect, the usual geometrical, or kinematical theory of diffraction is an insufficient approximation and the dynamical theory of diffraction must be used to describe the diffracted intensities.

3.10: Dynamical theory of Scattering

In the geometrical, or kinematical theory, the amplitudes diffracted by a three-dimensional periodic assembly of atoms (Laue) or by a stack of planes (Darwin) is derived by adding the amplitudes of the waves diffracted by each atom or by each plane, simply taking into account the optical path differences between them, but neglecting the interaction of the propagating waves and matter. This approximation is not compatible with the law of conservation of energy and is only valid for very small or highly imperfect crystals. The purpose of the dynamical theory is to take this interaction into account. There are three forms of the dynamical theory:

3.11: Electron density map

A three-dimensional description of the electron density in a crystal structure, determined from X-ray diffraction experiments. X-rays scatter from the electron clouds of atoms in the crystal lattice; the diffracted waves from scattering planes *h*,*k*,*l* are described by structure factors $\mathbf{F}_{hkl}$. The electron density as a function of position *x*,*y*,*z* is the Fourier transform of the structure factors:

$\rho(xyz) = \frac{1}{V} \sum_{hkl} F(hkl) \exp[-2\pi i (hx + ky + lz)]$.

The electron density map describes the contents of the unit cells averaged over the whole crystal and not the contents of a single unit cell (a distinction that is important where structural disorder is present).

Three-dimensional maps are often evaluated as parallel two-dimensional contoured sections at different heights in the unit cell.

Units

Electron density is measured in electrons per cubic ångström, e Å^{-3}.

Contributors

3.12: Ewald sphere

The Ewald sphere, or sphere of reflection, is a sphere of radius 1/λ passing through the origin *O* of the reciprocal lattice. The incident direction is along a radius of the sphere, **IO** (Figure 1). A reflected direction, of unit vector $\mathbf{s_h}$, will satisfy the diffraction condition if the diffraction vector **OH** = **IH** – **IO** = $\mathbf{s_h}/\lambda - \mathbf{s_o}/\lambda$ ($\mathbf{s_o}$ unit vector in the direction **IO**) is a reciprocal lattice vector, namely if *H* is a node of the reciprocal lattice (see Diffraction condition in reciprocal space) . If other reciprocal lattice nodes, such as *G*, lie also on the sphere, there will be reflected beams along **IG**, etc. This construction is known as the Ewald construction. When the wavelength is large, there are seldom more than two nodes, *O* and *H*, of the reciprocal lattice simultaneously on the Ewald sphere. When there are three or more, one speaks of multiple diffraction, multiple scattering or *n*-beam diffraction. This situation becomes increasingly frequent as the wavelength decreases and is practically routine for very short wavelengths such as those of γ-rays and electrons. The curvature of Ewald sphere then becomes negligible and it can often be approximated by a plane. Many reflections must then be taken into account at the same time.

When the wavelength changes, the radius of the Ewald sphere changes. If the incident beam is a white beam, with a wavelength range $\lambda_{min} \leq \lambda \leq \lambda_{max}$, there will be a nest of Ewald spheres of radii $1/\lambda_{max} \leq 1/\lambda \leq 1/\lambda_{min}$.

3.13: F(000)

The expression for a structure factor evaluated in the zeroth-order case $h = k = l = 0$ yields the result

$$F(000) = [(\sum f_{r})^{\,2} + (\sum f_{i})^{\,2}]^{1/2}$$

where f_r is the real part of the scattering factors at $\theta = 0^\circ$, f_i is the imaginary part of the scattering factors at $\theta = 0^\circ$, θ is the Bragg angle, and the sum is taken over each atom in the unit cell.

F(000) is computed without dispersion effects in electron-density calculation by Fourier inversion. In all cases, non-dispersive *F*(000) is a structure factor and not a structure amplitude: it has both magnitude and a sign.

For X-rays non-dispersive *F*(000) is positive definite and in many cases an integer (but it is not an integer for non-stoichiometric compounds). It counts the number of electrons in the cell.

For neutrons non-dispersive *F*(000) is either positive or negative and counts the total nuclear scattering power in the cell.

3.14: Friedel's Law

Friedel's law states that the intensities of the h, k, l and $\bar{h}, \bar{k}, \bar{l}$ reflections are equal. This is true either if the crystal is centrosymmetric or if no resonant scattering is present. It is in that case not possible to tell by diffraction whether an inversion center is present or not. The apparent symmetry of the crystal is then one of the eleven **Laue classes**.

The reason for Friedel's rule is that the diffracted intensity is proportional to the square of the modulus of the structure factor, $|F_h|^2$, according to the geometrical, or kinematical theory of diffraction. It depends similarly on the modulus of the structure factor according to the dynamical theory of diffraction. The structure factor is given by:

$$F_h = \sum_j f_j (exp - 2\pi i) \mathbf{h} \cdot \mathbf{r\_j}$$

where f_j is the atomic scattering factor of atom j, **h** the reflection vector and **r_j** the position vector of atom j. There comes:

$$|F_h|^2 = F_h F_h^* = F_h F_{\bar{h}} = |F_{\bar{h}}|^2$$

if the atomic scattering factor, f_j, is real. The intensities of the h, k, l and $\bar{h}, \bar{k}, \bar{l}$ reflections are then equal. If the crystal is absorbing, however, due to resonant scattering, the atomic scattering factor is complex and

$$F_{\bar{h}} \neq F_h^*$$

The reflections h, k, l and $\bar{h}, \bar{k}, \bar{l}$ are called a *Friedel pair*. They are used in the resolution of the phase problem for the solution of crystal structures and in the determination of absolute structure.

History

Friedel's law was stated by G. Friedel (1865-1933) in 1913 (Friedel G., 1913, *Sur les symétries cristallines que peut révéler la diffraction des rayons X.*, *C.R. Acad. Sci. Paris*, **157**, 1533-1536.

See also

Section 3.1 of *International Tables of crystallography, Volume A*

3.15: Friedel pair

The couple of reflections h, k, l and $\bar{h}, \bar{k}, \bar{l}$ is called a Friedel pair, or Bijvoet pair. Their intensities are equal either if the crystal structure is centrosymmetric or if there is no resonant scattering, but differ otherwise. Friedel's law then does not hold. For crystals with a non-centrosymmetric structure and significant resonant scattering, equivalent reflections generated by the symmetry operations of the point group of the crystal have intensities different from those of equivalent reflections generated by the introduction of an additional inversion centre in normal scattering. Friedel, or Bijvoet pairs are used in the resolution of the phase problem for the solution of crystal structures and in the determination of absolute structure.

3.16: Integral reflection conditions

The integral reflections are the general reflection conditions due to the centering of cells. They are given in the table below:

Integral reflection conditions for centered lattices.

Reflection condition	Centering type of cell	Centering symbol
None	Primitive	*P* *R* (rhombohedral axes)
$h + k = 2n$	*C*-face centered	*C*
$k + l = 2n$	*A*-face centered	*A*
$l + h = 2n$	*B*-face centered	*B*
$h + k + l = 2n$	body centered	*I*
$h + k$, $h + l$ and $k + l = 2n$ or: h, k, l all odd or all even (‘unmixed’)	all-face centered	*F*
$-h + k + l = 3n$	rhombohedrally centered, reverse setting	*R* (hexagonal axes)
$h - k + l = 3n$	rhombohedrally centered, obverse setting (standard)	
$h - k = 3n$	hexagonally centered	*H*

3.17: Kinematical theory

In the **kinematical** or **geometrical** theory, the amplitudes diffracted by a three-dimensional periodic assembly of atoms (Laue) or by a stack of planes (Darwin) is derived by adding the amplitudes of the waves diffracted by each atom or by each plane, simply taking into account the optical path differences between them, but neglecting the interaction of the propagating waves and matter. This approximation is not compatible with the law of conservation of energy and is only valid for very small or highly imperfect crystals. The purpose of the dynamical theory is to take this interaction into account .

3.18: Laue equations

The three Laue equations give the conditions to be satisfied by an incident wave to be diffracted by a crystal. Consider the three basis vectors, **OA** = **a**, **OB** = **b** , **OC** = **c** of the crystal and let $\vec{s}_o$ and $\vec{s}_h$ be unit vectors along the incident and reflected directions, respectively. The conditions that the waves scattered by *O* and *A*, *O* and *B*,*O* and *C*, respectively, be in phase are that

$$\vec{a}\cdot(\mathrm{s}_h-\vec{s}_o)=h\lambda$$

$$\vec{b}\cdot(\vec{s}_h-\vec{s}_o)=k\lambda$$

$$\vec{c}\cdot(\vec{s}_h-\vec{s}_o)=l\lambda$$

If these three conditions are simultaneously satisfied, the incoming wave is reflected on the set of lattice planes of Miller indices *h/n*, *k/n*, *l/n*. *h*, *k*, *l* are the indices of the reflection.

The three Laue equations can be generalized by saying that the diffraction condition is satisfied if the scalar product

$$\vec{r}\cdot(\vec{s}_h/\lambda-\vec{s}_o/\lambda)$$

is an integer for any vector

$$\vec{r}=u\vec{a}+v\vec{b}+w\vec{c}$$

where (u, v, w integers) of the direct lattice. This is the case if

$$(\mathbf{s_h}/\lambda - \mathbf{s_o}/\lambda) = h\,\mathbf{a^*} + k\,\mathbf{b^*} + l\,\mathbf{c^*},$$

where *h*, *k*, *l* are integers, namely if the diffraction vector **OH** = $\mathbf{s_h}$,/λ - $\mathbf{s_o}$/λ is a vector of the reciprocal lattice. This is the diffraction condition in reciprocal space.

History

The three Laue conditions for diffraction were first given in Laue, M. (1912). *Eine quantitative Prüfung der Theorie für die Interferenz-Erscheinungen bei Röntgenstrahlen*. *Sitzungsberichte der Kgl. Bayer. Akad. der Wiss* 363--373, reprinted in *Ann. Phys.* (1913), **41**, 989-1002 where he interpreted and indexed the first diffraction diagram (Friedrich, W., Knipping, P., and Laue, M. (1912). *Interferenz-Erscheinungen bei Röntgenstrahlen*, *Sitzungsberichte der Kgl. Bayer. Akad. der Wiss*, 303--322, reprinted in *Ann. Phys.*, (1913), **41**, 971-988, taken with zinc-blende, ZnS. For details, see P. P. Ewald, 1962, IUCr, 50 Years of X-ray Diffraction, Section 4, page 52.

Contributors

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  - Online Dictionary of Crystallography

3.19: Lorentz–polarization correction

A multiplicative factor involved in converting diffracted radiation intensities to structure factors during the process of structure determination for X-ray diffraction experiments involving moving crystals.

3.20: Mosaic crystal

The **mosaic crystal** is a simplified model of real crystals proposed by C. G. Darwin. In this model, a real crystal is described as a mosaic of crystalline blocks with dimensions of 10^{-5} cm, tilted to each other by fractions of a minute of arc. Each block is separated from the surrounding blocks by faults and cracks.

In a diffraction experiment, interference between waves only occurs inside a block, whose dimensions satisfy the theoretical conditions of applicability of the kinematical theory. Because of the loss of coherence between the waves diffracted from different blocks, the diffracted intensity from the whole crystal is equal to the sum of the intensities diffracted by every block.

3.21: Primary extinction

The **primary extinction** is responsible for the loss of intensity due to dynamic effect inside every block of a mosaic crystal. At the Bragg angle, each incident wave can undergo multiple reflections from different atomic planes; each scattering introduced causes a phase difference of λ/4 = π/2 so that along each direction waves differing by an even number of scattering, *i.e*. by nπ in phase, interfere , whose intensity decreasing rapidly with the number of scatterings. Because of the decrease in intensity of waves multiply scattered, the effect of waves differing by more than two scatterings can normally be neglected: in each direction one observes then the destructive interference between waves having a significant difference in intensity and an overall reduction of the intensity with respect to the intensity given by the kinematical theory.

3.22: Reflection conditions

The reflection conditions describe the conditions of occurrence of a reflection (structure factor not systematically zero). There are two types of systematic reflection conditions for diffraction of crystals by radiation:

(1) *General conditions*. They apply to all Wyckoff positions of a space group, *i.e.* they are always obeyed, irrespective of which Wyckoff positions are occupied by atoms in a particular crystal structure. They are due to one of three effects:

- *Centered cells*.

The resulting conditions apply to the whole three-dimensional set of reflections hkl. Accordingly, they are called *integral reflection conditions*. They are given in Table 1.

- *Glide planes*.

The resulting conditions apply only to two-dimensional sets of reflections, *i.e.* to reciprocal-lattice nets containing the origin (such as $hk0$, $h0l$, $0kl$, hhl). For this reason, they are called *zonal reflection conditions*. For instance, for a glide plane parallel to (001):

type of reflection	reflection condition	glide vector	glide plane
$0kl$	$k = 2n$	$\mathbf{b}/2$	b
	$l = 2n$	$\mathbf{c}/2$	c
	$k + l = 2n$	$\mathbf{b}/2 + \mathbf{c}/2$	n
	$k + l = 4n$ $k, l = 2n$	$\mathbf{b}/4 \pm \mathbf{c}/4$	d

The zonal reflection conditions are listed in Table 2.2.13.2 of *International Tables of Crystallography, Volume A*.

- *Screw axes*.

The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows containing the origin (such as $h00$, $0k0$, $00l$). They are called *serial reflection conditions*. For instance, for a screw axis parallel to [001], the reflection conditions are:

type of reflection	reflection condition	screw vector	screw axis
$00l$	$l = 2n$	$\mathbf{c}/2$	2_1; 4_2
	$l = 4n$	$\mathbf{c}/4$	4_1; 4_3
$000l$	$l = 2n$	$\mathbf{c}/2$	6_3
	$l = 3n$	$\mathbf{c}/3$	4_1; 3_1; 3_2; 6_2; 6_4
	$l = 6n$	$\mathbf{c}/6$	6_1;6_5

The serial reflection conditions are listed in Table 2.2.13.2 of *International Tables of Crystallography, Volume A*.

(2) *Special conditions* ('extra' conditions). They apply only to special Wyckoff positions and occur always in addition to the general conditions of the space group.

3.23: Resolution

In crystal structure determination, the term **resolution** is used to describe the ability to distinguish between neighboring features in an electron density map. By convention, it is defined as the minimum plane spacing given by Bragg's law for a particular set of X-ray diffraction intensities. The resolution improves with an increase in the maximum value of $(\sin\theta)/\lambda$ at which reflections are measured.

3.24: Resonant scattering

The elementary theory of the scattering of X-rays by atoms, leading to the real atomic scattering factor f_o, applies only for X-radiation whose wavelength is far removed from that of any natural (resonant) frequency of the atom. When this condition does not hold, one needs to use as physical model for the scattering that of a forced damped harmonic oscillator. This leads to resonant-scattering terms in the full, now complex, scattering factor of an atom, represented by:-

$$f = f_o + f\,' + i f\,'' \ .$$

The real and imaginary terms, $f\,'$, $f\,''$, in the atomic scattering factor are independent of sin(θ)/λ and in general small compared to f_o. The values of $f\,'$ and $f\,''$ change most at the absorption edge of the element in question.

In the older literature the term *anomalous dispersion* was used for resonant scattering. In macromolecular crystallography the term *anomalous scattering* is used widely in place of resonant scattering.

History

The resonant scattering of X-rays was theoretically predicted by Waller (Waller, I., 1928, *Über eine verallgemeinerte Streuungsformel*. *Z. Phys.* **51**, 213-231.) and first calculated by Hönl (Hönl, H., 1933, *Zur Dispersionstheorie der Röntgenstrahlen*. *Z. Phys.* **84**, 1-16; Hönl, H., 1933, *Atomfactor für Röntgenstrahlen als Problem der Dispersionstheorie (K-Schale)*. *Ann. Phys.* (Leipzig), **18**, 625-657.

Contributors

3.25: Secondary extinction

The **secondary extinction** is responsible for the loss of intensity occurring when the incident beam crosses a crystal. Each plane of a family (*hkl*) satisfying Laue equations (or Bragg's law) diffracts the incident beam, and thus subtracts part of the intensity to the incident beam. Successive planes of the same family will then experience a weakening of the incident beam and as a consequence the diffracted beams will result from the positive interference of waves not having the same intensities, as it is instead considered by the kinematical theory.

Secondary extinction is equivalent to an increase of the linear absorption coefficient and is negligible for sufficiently small crystals.

3.26: Serial reflection conditions

The serial reflection conditions are the general reflection conditions due to the presence of screw axes. The resulting conditions apply only to one-dimensional sets of reflections, *i.e.* reciprocal-lattice rows containing the origin (such as *h*00, 0*k*0, 00*l*). For instance, for a screw axis parallel to [001], the reflection conditions are:

type of reflection	reflection condition	screw vector	screw axis
00*l*	$l = 2n$	**c**/2	2_1; 4_2
	$l = 4n$	**c**/4	4_1; 4_3
000*l*	$l = 2n$	**c**/2	6_3
	$l = 3n$	**c**/3	4_1; 3_1; 3_2; 6_2; 6_4
	$l = 6n$	**c**/6	6_1;6_5

The serial reflection conditions are listed in Table 2.2.13.2 of *International Tables of Crystallography, Volume A*.

3.27: Structure Factor

The **structure factor F**$_{hkl}$ is a mathematical function describing the amplitude and phase of a wave diffracted from crystal lattice planes characterized by Miller indices h,k,l.

The structure factor may be expressed as

$$\mathbf{F}_{hkl} = F_{hkl}\exp(i\alpha_{hkl}) = \sum_j f_j \exp[2\pi i(hx_j + ky_j + lz_j)] \tag{3.27.1}$$

$$= \sum_j f_j \cos[2\pi(hx_j + ky_j + lz_j)] + i\sum_j f_j \sin[2\pi(hx_j + ky_j + lz_j)] \tag{3.27.2}$$

$$= A_{hkl} + iB_{hkl} \tag{3.27.3}$$

where the sum is over all atoms in the unit cell, x_j,y_j,z_j are the positional coordinates of the jth atom, f_j is the scattering factor of the jth atom, and α_{hkl} is the phase of the diffracted beam.

The intensity of a diffracted beam is directly related to the amplitude of the structure factor, but the phase must normally be deduced by indirect means. In structure determination, phases are estimated and an initial description of the positions and anisotropic displacements of the scattering atoms is deduced. From this initial model, structure factors are calculated and compared with those experimentally observed. Iterative refinement procedures attempt to minimize the difference between calculation and experiment, until a satisfactory fit has been obtained.

Derivation

Consider Bragg's law for an array of atom scatterers in a primitive lattice with just one atom at each lattice point. An incident X-ray wave of wavelength λ diffracts strongly through an angle 2θ where the perpendicular distance between two lattice planes d_{hkl} satisfies the relation

$$2d_{hkl}\sin\theta = n\lambda$$

It is seen that the path difference between waves diffracted from the two planes shown differs by just one wave cycle.

Now consider a second atom added to the unit cell. Each original atom is now accompanied by a companion atom of the new type, offset by a displacement vector $\mathbf{r}_1$. The incident X-ray beam will also diffract from these new scatterers (since they occupy planes parallel to those originally drawn). But now there is a phase difference φ_1 between the waves scattered from the first and the new sets of atoms.

The amplitudes of the waves are proportional to the atomic scattering factors f_0 and f_1. The phases differ by the angle φ_1 . The resultant vector represents the two-atom structure factor with amplitude F_{hkl}. Note that there is a net phase φ arising from the phase difference due to the offset in position between the two sets of diffracting atoms.

As in the case of two atoms, the resultant diffracted wave is obtained from the linear superposition of the wave vectors scattered from each different atom.

Units

The units of the structure-factor amplitude depend on the incident radiation. For X-ray crystallography they are multiples of the unit of scattering by a single electron ($2.82 \times 10^{-15}\ m$); for neutron scattering by atomic nuclei the unit of scattering length of $10^{-14}\ m$ is commonly used.

See also

The structure factor. P. Coppens. *International Tables for Crystallography* (2006). Vol. B, ch. 1.2, pp. 10-24

Contributors

3.28: Systematic absences

One speaks of *systematic absences* or *extinctions* when the structure factor is zero, due either to the centering of the lattice or to the presence of glide or screw symmetry elements. Conversely, the conditions for a reflection to exist and not to be systematically absent, are called reflection conditions.

3.29: Zonal reflection conditions

The zonal reflection conditions are the general reflection conditions due to the presence of glide planes. The resulting conditions apply only to two dimensional sets of reflections, *i.e.* to reciprocal-lattice nets containing the origin (such as *hk*0, *h*0*l*, 0*kl*, *hhl*). For instance, for a glide plane parallel to (001):

type of reflection	reflection condition	glide vector	glide plane
0*kl*	$k = 2n$	**b**/2	*b*
	$l = 2n$	**c**/2	*c*
	$k + l = 2n$	**b**/2 + **c**/2	*n*
	$k + l = 4n$ $k, l = 2n$	**b**/4 ± **c**/4	*d*

The zonal reflection conditions are listed in Table 2.2.13.2 of *International Tables of Crystallography, Volume A*.

CHAPTER OVERVIEW

4: Crystal Chemistry

4.1: Diadochy

Diadochy is the capability of an atom to replace another in a particular crystal structure. The degree of substitution depends on the physical conditions (temperature and pressure) as well as the atomic size, charge, and electronic structure of the diadochic partners.

4.2: Isomorphous Crystals

Two crystals are said to be isomorphous if (*a*) both have the same space group and unit-cell dimensions and (*b*) the types and the positions of atoms in both are the same except for a replacement of one or more atoms in one structure with different types of atoms in the other (isomorphous replacement), such as heavy atoms, or the presence of one or more additional atoms in one of them (*isomorphous addition*). Isomorphous crystals can form *solid solutions*.

4.3: Isostructural Crystals

Two crystals are said to be *isostructural* if they have the same structure, but not necessarily the same cell dimensions nor the same chemical composition, and with a 'comparable' variability in the atomic coordinates to that of the cell dimensions and chemical composition. For instance, calcite $CaCO_3$, sodium nitrate $NaNO_3$ and iron borate $FeBO_3$ are isostructural. One also speaks of *isostructural series*, or of *isostructural polymorphs* or *isostructural phase transitions*.

The term **isotypic** is synonymous with isostructural.

CHAPTER OVERVIEW

5: Structure Determination

Topic hierarchy

5.1: Bragg R factor

The *R* factor measuring the agreement between the reflection intensities calculated from a crystallographic model and those measured experimentally.

\(R_B =

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\).

In the Rietveld method R_B is useful because it depends on the fit of the structural parameters and not on the profile parameters.

5.2: Constrained refinement

A refinement is said to be constrained if one or more parameters in the refinement are held fixed or are determined by the value of one or more refined parameters. Constraints related to space group symmetry are not usually counted among the constraints applied to a given refinement as they are always present where applicable.

5.3: Direct methods

The family of methods for solving the phase problem in crystal structure determination. The phases of scattered diffraction beams cannot be directly observed. However, they can be estimated from probability relationships applied to the phases of the most intense diffraction peaks. The facts that scattering centers in a crystal are discrete atoms (*i.e.* sources of electron density) and that the electron density must be non-negative are the types of constraints that restrict the possible values of the phases, and allow initial estimates of some of them.

5.4: Free R factor

A residual function calculated during structure refinement in the same way as the conventional *R* factor, but applied to a small subset of reflections that are not used in the refinement of the structural model. The purpose is to monitor the progress of refinement and to check that the *R* factor is not being artificially reduced by the introduction of too many parameters.

5.5: Harker section

In Patterson methods of structure solution, relationships between symmetrically related atoms produce peaks in the Patterson function on certain planes or along certain lines determined by the known crystallographic symmetries. **Harker sections** are portions of the Patterson map that contain a large proportion of the readily interpretable information because they contain many such **Harker peaks** (vectors between space-group equivalent atoms).

Contributors

5.6: Heavy-Atom Method

An application of Patterson methods in crystal structure determination. For a compound containing a heavy atom (*i.e.* one with a significantly higher atomic scattering factor than the others present) the diffraction phases calculated from the position of the heavy atom are used to compute a first approximate electron density map. Further portions of the structure are recognizable as additional peaks in the map. Successive approximate electron density maps may then be calculated to solve the entire structure.

5.7: Phase problem

Waves diffracted from a primitive lattice of simple scatterers obey Bragg's law, which allows ready determination of interplanar distances and thus the easy recovery of a description of the crystal lattice. Where the scattering objects are complex (*e.g.* in molecular crystals) the diffracted radiation suffers a phase shift arising from the spatial distribution of individual scatterers. The amplitudes of the resulting structure factors are directly derivable from the experimental measured intensities of the diffracted beams, but the phases are not. Without a knowledge of the phases, it is not possible to reconstruct the individual atomic positions. Estimating the phases is an essential step in successful structure determination.

5.8: Refinement

In structure determination, the process of improving the parameters of an approximate (trial) structure until the best fit is achieved between an observed diffraction pattern and that calculated by Fourier transformation from the numerically parameterized trial structure.

5.9: Restrained refinement

A refinement is said to be restrained if the refinement is based on additional observations or pseudo-observations besides the observed structure factors.

5.10: Rietveld method

Method of analyzing powder diffraction data in which the crystal structure is refined by fitting the entire profile of the diffraction pattern to a calculated profile using a least-squares approach. There is no intermediate step of extracting structure factors, and so patterns containing many overlapping Bragg peaks can be analyzed.

5.11: R factor

The term ***R* factor** in crystallography is commonly taken to refer to the 'conventional' *R* factor

\(R =

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\),

a measure of agreement between the amplitudes of the structure factors calculated from a crystallographic model and those from the original X-ray diffraction data. The *R* factor is calculated during each cycle of least-squares structure refinement to assess progress. The final *R* factor is one measure of model quality.

More generally, a variety of *R* factors may be determined to measure analogous residuals during least-squares optimization procedures. Where the refinement attempts to minimize the deviates of the squares of the structure factors (refinement against F^2), the *R* factor based on F^2 is used to monitor the progress of refinement:

\(R(F^2) =

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\).

Likewise, refinement against *I* can be tracked using the Bragg *R* factor

\(R_B =

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\).

Even for refinement against F^2 or *I*, the 'conventional' *R* factor may be calculated and quoted as a measure of model quality, in order to compare the resulting quality of models calculated at different times and with different refinement strategies.

The *R* factor is sometimes described as the **discrepancy index**.

5.12: Sharpened Patterson function

Patterson methods of structure determination use the Patterson function

$P(uvw) = (1 / V)$	$\sum$	$\sum$	$\sum$	$\{ \mid F(hkl) \mid ^2 \cos[2\pi(hu + kv + lw)]\}$
	h	k	l	

to generate a map of interatomic vectors within the unit cell. Better results can be obtained by artificially sharpening the peaks in the Patterson function, thereby enhancing the resolution of individual peaks.

One technique for doing so, introduced by Patterson in 1935, considers the effect of thermal motion on the broadening of electron-density peaks and consequently their Patterson peaks. The F^2 coefficients can be corrected for thermal effects by simulating the atoms as point scatterers and using a modified set of coefficients $|\mathbf{F}_{\mathbf{h},\mathrm{sharp}}|^2 = |\mathbf{F}_{\mathbf{h}}|^2/\bar{f}^{-2}$, where $\bar{f}$, the average scattering factor per electron, is given by

$$\bar{f} = \sum_{i=1}^{N} f_i / \sum_{i=1}^{N} Z_i.$$

A common formulation for this type of sharpening expresses the atomic scattering factors at a given angle in terms of an overall isotropic thermal parameter B as $f(s) = f_0 \exp(-Bs^2)$. The Patterson coefficients then become

\(\mathbf{F}_{\mathbf{h}, \, \mathrm{sharp}} =

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\).

More often nowadays normalized structure factors $|E^2| - 1$ are used in place of $|F^2|$. Normalized structure factors are used in direct methods techniques of structure solution. They are defined as

$$|E_{\mathbf{h}}|^2 = |F_{\mathbf{h}}|^2 / \langle |F_{\mathbf{h}}|^2 \rangle,$$

where the squared observed structure-factor magnitudes on an absolute scale are divided by their expected values. Their use gives much greater weight to higher-resolution data and resolves some peaks in the vector map that would otherwise be continuous. On the other hand, they are less accurately known and are adjacent to data that have not been measured; they may therefore introduce spurious definition into the map.

A compromise that is often helpful is to use $|EF|$ as the Patterson coefficients.

5.13: Structure-factor coefficient

The quantity F, F^2 or I that is used in place of Y in the function $\sum w(Y_o - Y_c)^2$ minimized during least-squares refinement of a crystal structure determination.

5.14: Structure amplitude

The magnitude of the structure factor.

5.15: Structure determination

Structure determination in crystallography refers to the process of elaborating the three-dimensional positional coordinates (and also, usually, the three-dimensional anisotropic displacement parameters) of the scattering centers in an ordered crystal lattice. Where a crystal is composed of a molecular compound, the term generally includes the three-dimensional description of the *chemical* structures of each molecular compound present.

Experimental techniques

Owing to the highly ordered arrangement of atoms as scattering centers in a crystal lattice, most structure determination techniques involve the diffraction of electromagnetic or matter waves of wavelengths comparable to atomic dimensions. Bragg's law specifies the condition for plane waves to be diffracted from lattice planes. The diffracted radiation passing through a crystal emerges with intensity varying as a function of scattering angle. This variation arises from constructive and destructive interference of scattered beams from the planes associated with the different atoms present in the lattice. The result is seen by an imaging detector as a pattern of diffraction spots or rings.

Among diffraction-based techniques are:

- single-crystal X-ray diffraction
- X-ray powder diffraction
- X-ray fiber diffraction
- neutron powder diffraction
- neutron single-crystal diffraction
- polymer electron diffraction

Other techniques for three-dimensional structure determination that are complementary to diffraction methods include

- electron microscopy
- nuclear magnetic resonance spectroscopy (used largely for biological macromolecules in solution)

Methodology

The following summary applies to single-crystal X-ray diffraction. A crystal, mounted on a goniometer, is illuminated by a collimated monochromatic X-ray beam, and the positions and intensities of diffracted beams are measured. The measured intensities I_{hkl} (corresponding to scattering from a lattice plane with Miller indices h,k,l) are reduced to structure amplitudes F_{hkl} by the application of a number of experimental corrections:

$$F_{hkl}^2 = I_{hkl}(k\mathrm{Lp}A)^{-1}$$

where k is a scale factor, Lp the Lorentz–polarization correction, and A the transmission factor representing the absorption of X-rays by the crystal. The structure amplitude represents the amplitude of the diffracted wave measured relative to the scattering amplitude of a single electron.

However, the diffracted wave is completely described by the structure factor $\mathbf{F}_{hkl}$:

$$\mathbf{F}_{hkl} = F_{hkl}\exp(i\alpha_{hkl}) = \sum_j f_j\exp[2\pi i (hx_j + ky_j + lz_j)]$$

$$\qquad = \sum_j f_j\cos[2\pi (hx_j + ky_j + lz_j)] + i\sum_{j} f_j\sin[2\pi (hx_j + ky_j + lz_j)]$$

$$= A_{hkl} + iB_{hkl}$$

where the sum is over all atoms in the unit cell, x_j,y_j,z_j are the positional coordinates of the jth atom, f_j is the scattering factor of the jth atom, and α_{hkl} is the phase of the diffracted beam.

The atomic scattering factor can be worked out from the physical properties of the atom species, but the phase cannot be determined by direct experimental observation. If the phases can be derived in some way, then the positional coordinates can be calculated from the expression above. The phase problem represents the major obstacle to constructing an initial structural model, and is addressed through a number of techniques, such as direct methods, Patterson synthesis, heavy-atom method, isomorphous replacement *etc.*

Once an initial structural model has been calculated, it is usually necessary to conduct an iterative refinement procedure to improve the agreement between the structural model and the experimental diffraction intensities. The most common approach is to perform a least-squares minimization between the experimental structure factors and those calculated by varying the adjustable parameters of the structural model. These normally include atomic positions, anisotropic displacement parameters, occupancies, chemical bond lengths and angles, and other geometric characteristics of a molecule. Some metric, such as the residual R factor

\(R =

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\),

is used to indicate improvements or reductions in the quality of fit between model and observation. In the expression above (the 'conventional' R factor), F_{obs} and F_{calc} are the observed and calculated structure amplitudes, and the deviations are summed over all experimentally recorded intensities. There is considerable discussion on the most appropriate statistical metric to use for this purpose.

Other refinement techniques, such as maximum likelihood and maximum entropy, are also used.

5.16: Superposition methods

A subset of Patterson methods of structure solution that involve analyzing the Patterson map, transforming the origin of the map in turn on to the known positions of certain atoms, and suitably combining the superposed maps. The degree of coincidence between the peaks of the superposing maps is assessed by optimizing one of a number of image-seeking functions, of which the symmetry minimum function is perhaps most often used.

Contributors

CHAPTER OVERVIEW

6: Physical Properties of Crystals

Topic hierarchy

6.1: Atomic Scattering Factor

A measure of the scattering power of an isolated atom (also known as the **atomic form factor)**. The scattering factor depends on the scattering amplitude of an individual atom and also the Bragg angle of scattering. It depends on the type of radiation involved .

X-ray scattering

The scattering from a crystal of an X-ray beam results from the interaction between the electric component of the incident electromagnetic radiation and the electrons in the crystal. Tightly bound electrons scatter coherently (**Rayleigh scattering**); free electrons scatter incoherently (Compton scattering). The scattering process from atomic electrons in a crystal lattice has both coherent and incoherent components, and is described as Thomson scattering.

The scattering amplitude from a neutral atom depends on the number of electrons (\Z\) = the atomic number) and also on the Bragg angle θ – destructive interference among waves scattered from the individual electrons reduces the intensity at other than zero scattering angle. For $\theta = 0$ the scattering amplitude is normally equal to Z. However, the scattering factor is modified by anomalous scattering if the incident wavelength is near an absorption edge of the scattering element.

The X-ray scattering factor is evaluated as the Fourier transform of the electron density distribution of an atom or ion, which is calculated from theoretical wavefunctions for free atoms.

See also

1. Electron diffraction. C. Colliex, J. M. Cowley, S. L. Dudarev, M. Fink, J. Gjønnes, R. Hilderbrandt, A. Howie, D. F. Lynch, L. M. Peng, G. Ren, A. W. Ross, V. H. Smith Jr, J. C. H. Spence, J. W. Steeds, J. Wang, M. J. Whelan and B. B. Zvyagin. *International Tables for Crystallography*(2006). Vol. C, ch. 4.3, pp. 259-429
2. Intensity of diffracted intensities. P. J. Brown, A. G. Fox, E. N. Maslen, M. A. O'Keefe and B. T. M. Willis. *International Tables for Crystallography* (2006). Vol. C, ch. 6.1, pp. 554-595
3. Neutron techniques. I. S. Anderson, P. J. Brown, J. M. Carpenter, G. Lander, R. Pynn, J. M. Rowe, O. Schärpf, V. F. Sears and B. T. M. Willis. *International Tables for Crystallography* (2006). Vol. C, ch. 4.4, pp. 430-487

Contributors

6.2: Curie laws

Curie extended the notion of symmetry to include that of physical phenomena and stated that:

- the symmetry characteristic of a phenomenon is the highest compatible with the existence of the phenomenon;
- the phenomenon may exist in a medium which possesses that symmetry or that of a subgroup of that symmetry.

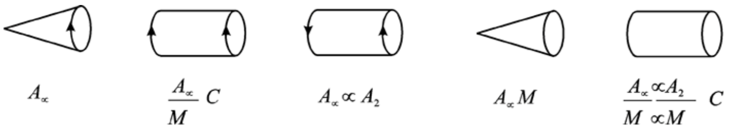
and concludes that some symmetry elements may coexist with the phenomenon but that their presence is not necessary. On the contrary, what is necessary is the absence of certain symmetry elements: ‘asymmetry creates the phenomenon’. Noting that physical phenomena usually express relations between a cause and an effect (an influence and a response), P. Curie restated the two above propositions in the following way, now known as Curie laws, although they are not, strictly speaking, laws (Curie himself spoke about 'the principle of symmetry'):

- the asymmetry of the effects must pre-exist in the causes;
- the effects may be more symmetric than the causes.

6.3: Cylindrical system

The cylindrical system contains non-crystallographic point groups with one axis of revolution (or isotropy axis). There are five groups in the spherical system:

Hermann-Mauguin symbol	Short Hermann-Mauguin symbol	Schönfliess symbol	order of the group	general form
A_∞	∞	C_∞	∞	rotating cone
$\frac{A_\infty}{M}C$	$\bar{\infty}$	$C_{\infty\,h} \equiv S_\infty \equiv C_{\infty\,i}$	∞	rotating finite cylinder
$A_\infty \infty\, A_2$	$\infty 2$	D_∞	∞	finite cylinder submitted to equal and opposite torques
$A_\infty M$	$\infty\, m$	$C_{\infty\,v}$	∞	stationary cone
$\frac{A_\infty}{M}\frac{\infty\,A_2}{\infty\,M}C$	$\bar{\infty}\, m \equiv \bar{\infty}\frac{2}{m}$	$D_{\infty\,h} \equiv D_{\infty\,d}$	∞	stationary finite cylinder



Note that $A_\infty M$ represents the symmetry of a force, or of an electric field and that $\frac{A_\infty}{M}C$ represents the symmetry of a magnetic field (Curie 1894), while $\frac{A_\infty}{M}\frac{\infty\,A_2}{\infty\,M}C$ represents the symmetry of a uniaxial compression.

6.4: Dual basis

The dual basis is a basis associated to the basis of a vector space. In three-dimensional space, it is isomorphous to the basis of the reciprocal lattice. It is mathematically defined as follows:

Given a basis of n vectors $\mathbf{e_i}$ spanning the direct space E^n, and a vector $\mathbf{x} = x^i\, \mathbf{e_i}$, let us consider the n quantities defined by the scalar products of $\mathbf{x}$ with the basis vectors, $\mathbf{e_i}$:

$$x_i = \mathbf{x} \,.\, \mathbf{e_i} = x^j\, \mathbf{e_j} \,.\, \mathbf{e_i} = x^j\, g_{ji},$$

where the g_{ji} 's are the doubly covariant components of the metric tensor.

By solving these equations in terms of x^j, one gets:

$$x^j = x_i\, g^{ij}$$

where the matrix of the g^{ij} 's is inverse of that of the g_{ij} 's ($g^{ik} g_{jk} = \delta^{\mathrm{i}}{}_{\mathrm{j}}$). The development of vector $\mathbf{x}$ with respect to basis vectors $\mathbf{e_i}$ can now also be written:

$$\mathbf{x} = x^i\, \mathbf{e_i} = x_i\, g^{ij}\, \mathbf{e_j}$$

The set of n vectors $\mathbf{e^i} = g^{ij}\, \mathbf{e_j}$ that span the space E^n forms a basis since vector $\mathbf{x}$ can be written:

$$\mathbf{x} = x_i\, \mathbf{e^i}$$

This basis is the *dual basis* and the n quantities x_i defined above are the coordinates of $\mathbf{x}$ with respect to the dual basis. In a similar way one can express the direct basis vectors in terms of the dual basis vectors:

$$\mathbf{e_i} = g_{ij}\, \mathbf{e^j}$$

The scalar products of the basis vectors of the dual and direct bases are:

$$g^i{}_j = \mathbf{e^i} \,.\, \mathbf{e_j} = g^{ik}\, \mathbf{e_k} \,.\, \mathbf{e_j} = g^{ik} g_{jk} = \delta^{\mathrm{i}}{}_{\mathrm{j}}.$$

One has therefore, since the matrices g^{ik} and g_{ij} are inverse:

$$g^i{}_j = \mathbf{e^i} \,.\, \mathbf{e_j} = \delta^{\mathrm{i}}{}_{\mathrm{j}}.$$

These relations show that the dual basis vectors satisfy the definition conditions of the reciprocal vectors. In a three-dimensional space the dual basis and the basis of reciprocal space are identical.

6.5: Electrocaloric effect

The electrocaloric effect is the converse of the pyroelectric effect: it describes the variation of entropy $\delta\sigma$ of a material submitted to an applied electrical field E_i :

$$\delta\sigma = p_i^T E_i$$

where p_i^T is the electrocaloric coefficient at constant stress. It is equal to the pyroelectric coefficient.

6.6: Metric tensor

A metric tensor is used to measure distances in a space. In crystallography the spaces considered are vector spaces with *Euclidean* metrics, *i.e.*ones for which the rules of Euclidean geometry apply. In that case, given a basis $\mathbf{e_i}$ of a *Euclidean space*, E^n, the metric tensor is a rank 2 tensor the components of which are:

$$g_{ij} = \mathbf{e_i} \,.\, \mathbf{e_j} = \mathbf{e_j}.\mathbf{e_i} = g_{ji}.$$

It is a symmetrical tensor. Using the metric tensor, the scalar product of two vectors, $\mathbf{x} = x^i\,\mathbf{e_i}$ and $\mathbf{y} = y^j\,\mathbf{e_j}$ is written:

$$\mathbf{x} \,.\, \mathbf{y} = x^i\,\mathbf{e_i} \,.\, y^j\,\mathbf{e_j} = g_{ij}\,x^i\,y^j.$$

In a three-dimensional space with basis vectors **a**, **b**, **c**, the coefficients g_{ij} of the metric tensor are:

$$g_{11} = \mathbf{a}^2;\ g_{12} = \mathbf{a} \,.\, \mathbf{b};\ g_{13} = \mathbf{a} \,.\, \mathbf{c};$$
$$g_{21} = \mathbf{b} \,.\, \mathbf{a};\ g_{22} = \mathbf{b}^2;\ g_{23} = \mathbf{b} \,.\, \mathbf{c};$$
$$g_{31} = \mathbf{c} \,.\, \mathbf{a};\ g_{32} = \mathbf{c} \,.\, \mathbf{b};\ g_{33} = \mathbf{c}^2;$$

Because the metric tensor is symmetric, $g_{12} = g_{21}$, $g_{13} = g_{31}$, and $g_{13} = g_{31}$. Thus there are only six unique elements, often presented as

$$g_{11}\ g_{22}\ g_{33}$$
$$g_{23}\ g_{13}\ g_{12}$$

or, multiplying the second row by 2, as a so-called G^6 ("G" for Gruber) vector

$$(\ \mathbf{a}^2, \mathbf{b}^2, \mathbf{c}^2, 2\ \mathbf{b} \,.\, \mathbf{c}, 2\ \mathbf{a} \,.\, \mathbf{c}, 2\ \mathbf{a} \,.\, \mathbf{b}\ )$$

The inverse matrix of g_{ij}, g^{ij}, ($g^{ik}g_{kj} = \delta^k{}_j$, Kronecker symbol, = 0 if $i \neq j$, = 1 if $i = j$) relates the dual basis, or reciprocal space vectors $\mathbf{e^i}$ to the direct basis vectors $\mathbf{e_i}$ through the relations:

$$\mathbf{e^j} = g^{ij}\ \mathbf{e_j}$$

In three-dimensional space, the dual basis vectors are identical to the reciprocal space vectors and the components of g^{ij} are:

$$g^{11} = \mathbf{a}^{*2};\ g^{12} = \mathbf{a}^* \,.\, \mathbf{b}^*;\ g^{13} = \mathbf{a}^* \,.\, \mathbf{c}^*;$$
$$g^{21} = \mathbf{b}^* \,.\, \mathbf{a}^*;\ g^{22} = \mathbf{b}^{*2};\ g^{23} = \mathbf{b}^* \,.\, \mathbf{c}^*;$$
$$g^{31} = \mathbf{c}^* \,.\, \mathbf{a}^*;\ g^{32} = \mathbf{c}^* \,.\, \mathbf{b}^*;\ g^{33} = \mathbf{c}^{*2};$$

with:

$$g^{11} = b^2c^2 \sin^2 \alpha/\ V^2;\ g^{22} = c^2a^2 \sin^2 \beta/\ V^2;\ g^{33} = a^2b^2 \sin^2 \gamma/\ V^2;$$

$$g^{12} = g^{21} = (abc^2/\ V^2)(\cos\alpha \cos\beta - \cos\gamma);\ g^{23} = g^{32} = (a^2bc/\ V^2)(\cos\beta \cos\gamma - \cos\alpha);\ g^{31} = g^{13} = (ab^2c/\ V^2)(\cos\gamma \cos\alpha - \cos\beta)$$

where V is the volume of the unit cell (**a**, **b**, **c**).

Change of basis

In a change of basis the direct basis vectors and coordinates transform like:

$$\mathbf{e'_j} = A_j{}^i\ \mathbf{e_i};\ x'^j = B_i{}^j\ x^i,$$

where $A_j{}^i$ and $B_i{}^j$ are transformation matrices, transpose of one another. According to their definition, the components g_{ij}, of the metric tensor transform like products of basis vectors:

$$g'_{kl} = A_k{}^iA_l{}^jg_{ij}.$$

They are the doubly covariant components of the metric tensor.

The dual basis vectors and coordinates transform in the change of basis according to:

$$\mathbf{e'^j} = B_i{}^j\ \mathbf{e^i};\ x'_j = A_j{}^i x_i,$$

and the components g^{ij} transform like products of dual basis vectors:

$g'^{kl} = A_i{}^k\ A_j{}^l\ g^{ij}.$

They are the doubly contravariant components of the metric tensor.

The mixed components, $g^i_j = \delta^i_j$, are once covariant and once contravariant and are invariant.

Properties of the metric tensor

- The **tensor nature** of the metric tensor is demonstrated by the behaviour of its components in a change of basis. The components g_{ij} and g^{ij} are the components of a *unique* tensor.
- The **squares of the volumes** *V* and *V** of the direct space and reciprocal space unit cells are respectively equal to the determinants of the g_{ij} 's and the g^{ij} 's:

$$V^2 = \Delta (g_{ij}) = abc(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \alpha \cos \alpha)$$

$$V^{*2} = \Delta (g^{ij}) = 1/ V^2.$$

- One changes the **variance of a tensor** by taking the contracted tensor product of the tensor by the suitable form of the metric tensor. For instance:

$$g_{im} t^{ij..}{}_{kl..} = t^{j..}{}_{klm..}$$

Multiplying by the doubly covariant form of the metric tensor increases the covariance by one, multiplying by the doubly contravariant form increases the contravariance by one.

See also

- Section 1.1.3 of *International Tables of Crystallography, Volume B*
- Section 1.1.2 of *International Tables of Crystallography, Volume D*

Contributors

6.7: Neumann's Principle

Neumann's principle, or principle of symmetry, states that, if a crystal is invariant with respect to certain symmetry elements, any of its physical properties must also be invariant with respect to the same symmetry elements, or otherwise stated, the symmetry elements of any physical property of a crystal must include the symmetry elements of the point group of the crystal. It is generalized to physical phenomena by Curie laws.

6.8: Piezoelectricity

Piezoelectricity is the property presented by certain materials that exhibit an electric polarization when submitted to an applied mechanical stress such as a uniaxial compression. Conversely, their shape changes when they are submitted to an external electric field; this is the converse piezoelectric effect. The piezoelectric effect and the converse effect are described by third-rank tensors:

- For a small stress, represented by a second-rank tensor, T_{ij}, the resulting polarization, of components P_k , is given by:

$P_k = d_{kij} T_{ij}$

where d_{kij} is a third-rank tensor representing the direct piezoelectric effect.

- For a small applied electric field, of components E_k, the resulting strain, represented by a second-rank tensor, S_{ij}, is given by:

$S_{ij} = d_{ijk} E_k + Q_{ijkl} E_k E_l$

where the first-order term, d_{ijk}, represents the inverse piezoelectric effect and the second-order term, Q_{ijkl}, a symmetric fourth-rank tensor, the electrostriction effect. The sense of the strain due to the piezoelectric effect changes when the sign of the applied electric field changes , while that due to electrostriction, a quadratic effect, does not.

The matrices associated to the coefficients d_{kij} and d_{kij} of the direct and converse piezoelectric effects, respectively, are transpose of one another.

6.9: Pyroelectricity

Pyroelectricity is the property presented by certain materials that exhibit an electric polarization P_i when a temperature variation $\delta\Theta$ is applied uniformly:

$$P_i = p_i^T\ \delta\Theta$$

where p_i^T is the pyroelectric coefficient at constant stress. Pyroelectric crystals actually have a spontaneous polarization, but the pyroelectric effect can only be observed during a temperature change. If the polarization can be reversed by the application of an electric field, the crystal is ferroelectric.

If the crystal is also piezoelectric, the polarization due to an applied temperature variation is also partly due to the piezoelectric effect. The coefficient describing the pure pyroelectric effect is the pyroelectric coefficient at constant strain, p_i^S. The two coefficients are related by:

$$p_i^T = c_{ijkl} d_{kln} \alpha_{jn} + p_i^S$$

where the c_{ijkl} are the elastic stiffnesses, the d_{kln} the piezoelectric coefficients and the α_{jn} the linear thermal expansion coefficients.

The converse effect is the electrocaloric effect. If a pyroelectric crystal is submitted to an electric field, it will undergo a change of entropy $\Delta\sigma$:

$\Delta\sigma = p_i\ E^i$

and will release or absorb a quantity of heat given by $\Theta\ V\ \Delta\sigma$ where Θ is the temperature of the specimen and V its volume.

6.10: Spherical Systems

The spherical system contains non-crystallographic point groups with more than one axis of revolution. These groups, therefore, contain an infinity of axes of revolution (or isotropy axis). There are two groups in the spherical system:

Hermann-Mauguin symbol	Short Hermann-Mauguin symbol	Schönfliess symbol	order of the group	general form
∞A_∞	2∞	K	∞	sphere filled with an optically active liquid
$\infty \frac{A_\infty}{M} C$	$m\bar{\infty}, \frac{2}{m}\bar{\infty}$	K_h	∞	stationary sphere

History

The groups containing isotropy axes were introduced by P. Curie (1859-1906) in order to describe the symmetry of physical systems (Curie P. (1884). *Sur les questions d'ordre: répétitions. Bull. Soc. Fr. Minéral.*, **7**, 89-110; Curie P. (1894). *Sur la symétrie dans les phénomènes physiques, symétrie d'un champ électrique et d'un champ magnétique. J. Phys. (Paris)*, **3**, 393-415.).

See also

Section 10.1.4 of *International Tables of Crystallography, Volume A*
Section 1.1.4 of *International Tables of Crystallography, Volume D*

6.11: Thermal expansion

CHAPTER OVERVIEW

7: Morphological Crystallography

7.1: Law of Rational Indices

The law of rational indices states that the intercepts, *OP*, *OQ*, *OR*, of the natural faces of a crystal form with the unit-cell axes **a**, **b**, **c** (see Figure 1) are inversely proportional to prime integers, *h*, *k*, *l*. They are called the Miller indices of the face. They are usually small because the corresponding lattice planes are among the densest and have therefore a high interplanar spacing and low indices.

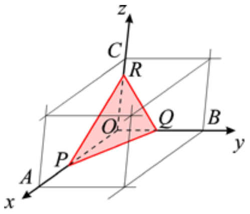
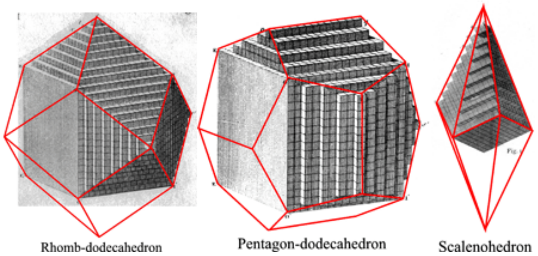


Figure 1

The law of rational indices was deduced by Haüy (1784, 1801) from the observation of the stacking laws required to build the natural faces of crystals by piling up elementary blocks, for instance cubes to construct the {110} faces of the rhomb-dodecahedron observed in garnets or the ½{210} faces of the pentagon-dodecahedron observed in pyrite, or rhombohedrons to construct the {21.1} (referred to an hexagonal lattice, $\{2\bar{1}0\}$, referred to a rhombohedral lattice) scalenohedron of calcite.



Rhomb-dodecahedron Pentagon-dodecahedron Scalenohedron

(Models from Haüy's *Traité de Minéralogie* (1801) - the crystal forms have been redrawn in red).

7.2: Law of the constancy of interfacial angles

The law of the constancy of interfacial angles (or 'first law of crystallography') states that the angles between the crystal faces of a given species are constant, whatever the lateral extension of these faces and the origin of the crystal, and are characteristic of that species. It paved the way for Haüy's law of rational indices.

7.3: Polar Lattice

The **polar lattice** is a lattice dual of the direct lattice, which is the ancestor of the reciprocal lattice. It was introduced by Auguste Bravais in a " mémoire" presented to the *Académie de Sciences de Paris* on 11 December 1848.

The construction of the polar lattice is essentially the same as that of the reciprocal lattice, but the parameter along a row of the polar lattice is $V^{2/3}/d(hkl)$ instead of $1/d(hkl)$. The polar lattice has thus the same dimensions as the direct lattice, namely Ångstroms, instead of Ångstroms^{-1}, like the reciprocal lattice.

- The unit cell of the polar lattice has the same volume as that of the direct lattice.
- The scalar product of the basis vectors of the direct and polar lattice is $V^{2/3}\delta_{ij}$, where δ is **Kroneker's tensor** and the indices i and j point to the basis vectors.

The polar lattice was introduced to facilitate the morphological study of crystals.

7.4: Zone axis

A zone axis is a lattice row parallel to the intersection of two (or more) families of lattices planes. It is denoted by [*u v w*]. A zone axis [*u v w*] is parallel to a family of lattice planes of Miller indices (*hkl*) if:

$$uh + vk + wl = 0$$

This is the so-called Weiss law.

The indices of the zone axis defined by two lattice planes (h_1,k_1,l_1), (h_2,k_2,l_2) are given by:

$$\frac{u}{\begin{vmatrix} k_1 & l_1 \\ k_2 & l_2 \end{vmatrix}} = \frac{v}{\begin{vmatrix} l_1 & h_1 \\ l_2 & h_2 \end{vmatrix}} = \frac{w}{\begin{vmatrix} h_1 & k_1 \\ h_2 & k_2 \end{vmatrix}}$$

Conversely, any crystal face can be determined if one knows two zone axes parallel to it. It is the zone law, or *Zonenverbandgesetz*.

Three lattice planes have a common zone axis (*are in zone*) if their Miller indices (h_1,k_1,l_1), (h_2,k_2,l_2), (h_3,k_3,l_3) satisfy the relation:

\begin{vmatrix} h_1 & k_1 & l_1\\ h_2 & k_2 & l_2\\ h_3 & k_3 & l_3\\ \end{vmatrix} = 0

$$\begin{vmatrix} h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 \\ h_3 & k_3 & l_3 \end{vmatrix} = 0$$

CHAPTER OVERVIEW

8: Powder Diffraction

Powder diffraction uses X-ray, neutron, or electron diffraction on powder or microcrystalline samples for structural characterization.

Topic hierarchy

8.1: Preferred orientation

Preferred orientation arises when there is a stronger tendency for the crystallites in a powder or a texture to be oriented more one way, or one set of ways, than all others. An easily visualized case of preferred orientation is that which results when a material with a strong cleavage or growth habit is packed into a specimen or when a metal sheet is obtained by rolling.

Preferred orientation should not be confused with 'graininess' or 'inadequate powder average', in which there are so few crystallites being irradiated that the number of correctly oriented crystallites varies significantly from reflection to reflection of different types.

CHAPTER OVERVIEW

9: Twinning

Crystal twinning occurs when two separate crystals share some of the same crystal lattice points in a symmetrical manner. The result is an intergrowth of two separate crystals in a variety of specific configurations.

9.1: Allotwin

An **allotwin** is a twin whose individuals are different polytypes of the same compound.

Contributors

9.2: Corresponding Twins

In case of twinning by merohedry, when the twin element is twofold and the crystal is centrosymmetric, the twin operation can be described either as a rotation or as a reflection (the two operations being equivalent under the action of the center).

In case of twinning by pseudomerohedry, instead, the two twin operations are no longer equivalent even in centrosymmetric crystals but produce different twins, which are called **reciprocal twins** (Mügge, 1898) or **corresponding twins** (Friedel, 1904, 1926). One of the most classical examples is that of albite vs. pericline twins in feldspars.

Pairs of corresponding twins normally do not have the same frequency of occurrence, as one would be tempted to assume from the identical value of their twin obliquity.

9.3: Hybrid twin

A twin in which more than one concurrent sublattice is necessary to explain the restoration of lattice nodes by the twin operation is called a **hybrid twin**.

Contributors

9.4: Inversion twin

Two domains of one crystal form an *inversion twin* when the twin operation is an inversion through a center (*twin center*).

Contributors

9.5: Mallard's Law

The **law of Mallard** was introduced by Georges Friedel (*Leçons de Cristallographie* 1926, page 436) to explain, on reticular basis, twinning by pseudomerohedry.

The law of Mallard states that twin elements are always rational (i.e. direct lattice elements): therefore, a twin plane is a lattice plane, and a twin axis is a lattice row. These twin elements are pseudosymmetry elements for the lattice of the individual. The twin operations produce now slightly different orientations of the lattice of the individual, which are only quasi-equivalent, and no longer equivalent, as in the case of twinning by merohedry.

9.6: Reflection twin

Two domains of one crystal form a *reflection twin* when the twin operation is a reflection across a lattice plane (*twin plane*).

Contributors

9.7: Rotation Twin

Two domains of one crystal form a *rotation twin* when the twin operation is a rotation about a lattice row (*twin axis*).

9.8: Selective merohedry

In twinning by merohedry, the twin operations belong to the point group of the crystal lattice. When twinning concerns an OD structure, the definition of merohedry should take into account not only the point group of the crystal and that of the lattice, but also the point group of the family structure. If the latter is a subgroup of the twin point group, some of the twin laws restore only a part of the reciprocal lattice nodes corresponding to the family reflections (the reflections common to all the OD structures of a family). This kind of twinning is called **twinning by selective merohedry**: it can occur when the Laue point group of the crystal is lower than the twin point group, *i.e*. in the so-called “class II twins”.

Contributors

9.9: TLQS twinning

TLQS (Twin Lattice Quasi-Symmetry) twinning is a term employed to indicate twinning where the twin lattice is close to a higher holohedry. The degree of quasi-symmetry is commonly measure by the twin obliquity, which depends on the perpendicularity of lattice row / lattice plane [*uvw*] / (*hkl*) defining the cell of the twin lattice.

9.10: TLS twinning

TLS (Twin Lattice Symmetry) twinning is a term employed to indicate twinning where the twin lattice does not possess a pseudo-symmetry, differently from what happens in TLQS twinning.

In TLS twinning, the lattice row / lattice plane [*uvw*] / (*hkl*) defining the cell of the twin lattice are mutually perpendicular. When this perpendicularity is imposed by the symmetry of the lattice, one speaks of *intrinsic-TLS* (*i-TLS*). In all other cases, the conditions of perpendicularity, depend on one or more metric parameters: one then speaks of *extrinsic-TLS* (*e-TLS*).

9.11: Twinning

9.12: Twinning(effects of)

9.13: Twinning (consequences of)

By effect of a twinning operation, both the direct and reciprocal lattice of the individuals forming a twin are overlapped. Overlapping (restoration) of nodes belonging to different individuals can be: (i) exact and total (twinning by merohedry); (ii) exact but partial (i.e. only a fraction of the nodes of an individual lattice is restored; twinning by reticular merohedry); (iii) total but approximate (twinning by pseudomerohedry), approximate and partial (twinning by reticular pseudomerohedry).

- **twin index**

The reciprocal n of the fraction $1/n$ of (quasi)restored nodes is called *twin index*

- **twin lattice**

The lattice that is formed by the (quasi)restored nodes is the *twin lattice*. It corresponds to the crystal lattice in twins by (pseudo)merohedry and to a sublattice of the crystal (individual) in twins by reticular (pseudo)merohedry.

- **twin obliquity**

The *twin obliquity* is a measure of the distortion of a (sub)lattice in twins by (reticular) pseudomerohedry.

9.14: Twinning (endemic conditions of)

When a lattice necessarily contains at least one sublattice that supports either twinning by reticular merohedry or twinning by reticular pseudomerohedry, it is said that an endemic condition of twinning does exist. The following cases are known.

9.15: Twinning by inversion

The symmetry operation relating pairs of domain structures twinned by inversion may be represented by inversion through a point or by some other isometry equivalent to inversion under the point symmetry group of the domain structure. A two-domain-structure twin that is twinned by inversion is called an *inversion twin*, but this term is not appropriate when there are more than two domain structures. Twinning by inversion can only occur in non-centrosymmetric structures.

9.16: Twinning by merohedry

The twin operation belongs to to the point group of the lattice but not to the point group of the crystal. Therefore, the point group of the crystal must be a subgroup of the point group of the lattice, i.e. the crystal shows only a part (*merohedry*) of the symmetry elements belonging to the its lattice which, instead, shows *holohedry* (complete symmetry). The twinning element of symmetry may (*Class I of twins by merohedry*) or may not belong to the Laue class of the crystal (*Class II of twins by merohedry*): Examples - Class I: in crystals with point group 2 (Laue group 2/*m*) the mirror plane *m* acts as twinning operator . Class II: in crystals with point group 4 (Laue group 4/*m*) a mirror plane *m* parallel to the foufold axis 4 acts as twinning operator.

9.17: Twinning by metric merohedry

Twinning by metric merohedry is a special case of twinning by merohedry which occurs when:

- the lattice of the individual has accidentally a specialized metric which corresponds to a higher holohedry
- the twin operation belongs to this higher holohedry only

If H is the individual point group, D(H) the corresponding holohedry and D(L) the point group of the lattice, twinning by metric merohedry corresponds to $D(L) \supset D(H) \supseteq H$

Twinning by metric merohedry can be seen as the degeneration of twinning by reticular merohedry to twin index 1, or of twinning by pseudomerohedry to twin obliquity zero.

9.18: Twinning by psuedomerohedry

A lattice is said to be pseudosymmetric if at least a lattice row or/and a lattice plane approximately correspond to elements of symmetry; these elements can act as twinning operators (e.g., a monoclinic lattice with its oblique angle *close* to 90° is pseudo-orthorhombic and thus shows two pseudo twofold axes and two pseudo mirror planes).

Chapter 3.3 of *International Tables of Crystallography, Volume D*

9.19: Twinning by reticular merohedry

In the presence of a sublattice whose oriented point group D($\mathbf{L}_{\mathrm{T}}$) differs from that of the crystal (individual) lattice D($\mathbf{L}_{\mathrm{ind}}$), a symmetry element belonging to D($\mathbf{L}_{\mathrm{T}}$) but not to D($\mathbf{L}_{\mathrm{ind}}$) can act as twin element.

If lattice and sublattice have the same point group but (some of) their symmetry elements are differently oriented, *twinning by reticular polyholohedry* can occur.

9.20: Twinning by reticular polyholohedry

Twinning by **reticular polyholohedry** is a special case of twinning by reticular merohedry that occurs when the twin lattice has the same point group as the lattice of the individual but at least one of its symmetry elements is differently oriented in space.

When the point group of the twin lattice is only close to that of the individual lattice one speaks of **twinning by reticular pseudopolyholohedry**, which corresponds to non-zero twin obliquity.

9.21: Twinning by reticular pseudomerohedry

In the presence of a sublattice displaying pseudosymmetry, a pseudosymmetry element belonging to the sublattice can act as twinning operator. See twinning by pseudomerohedry and twinning by reticular merohedry.

Chapter 3.3 of *International Tables of Crystallography, Volume D*

9.22: Twin element

The direct lattice element about which a twin operation is performed.

9.23: Twin index

A twin operation overlaps both the direct and reciprocal lattices of the individuals that form a twin; consequently, the nodes of the individual lattices are overlapped (restored) to some extent (twinning). The reciprocal *n* of the fraction 1/*n* of (quasi)restored nodes is called *twin index*

Let (*hkl*) be the twin plane and [*uvw*] the lattice direction (quasi)-normal to it. alternatively, let [*uvw*] be the twin axis and (*hkl*) the lattice plane (quasi)-normal to it. For *twofold operations*(180º rotations or reflections) the twin index is:

$n = X/\mathrm{f}$, $X = |uh+vk+wl|$

where f depends on the lattice type and on the parities of *X*, *h*, *k*, *l*, *u*, *v* and *w*, as in the following table

Lattice type	condition on *hkl*	condition on *uvw*	condition on *X*	*n*
P	none	none	X odd	*n* = *X*
			X even	*n* = *X*/2
C	*h*+*k* odd	none	none	*n* = *X*
	h+*k* even	*u*+*v* and *w* not both even	*X* odd	*n* = *X*
			X even	*n* = *X*/2
		u+*v* and *w* both even	*X*/2 odd	*n* = *X*/2
			X/2 even	*n* = *X*/4
B	*h*+*l* odd	none	none	*n* = *X*
	h+*l* even	*u*+*w* and *v* not both even	*X* odd	*n* = *X*
			X even	*n* = *X*/2
		u+*w* and *v* both even	*X*/2 odd	*n* = *X*/2
			X/2 even	*n* = *X*/4
A	*k*+*l* odd	none	none	*n* = *X*
	k+*l* even	*v*+*w* and *u* not both even	*X* odd	*n* = *X*
			X even	*n* = *X*/2
		v+*w* and *u* both even	*X*/2 odd	*n* = *X*/2
			X/2 even	*n* = *X*/4
I	*h*+*k*+*l* odd	none	none	*n* = *X*
	h+*k*+*l* even	*u*, *v* and *w* not all odd	*X* odd	*n* = *X*
			X even	*n* = *X*/2
		u, *v* and *w* all odd	*X*/2 odd	*n* = *X*/2
			X/2 even	*n* = *X*/4
F	none	*u*+*v*+*w* odd	none	*n* = *X*
h, *k*, *l* not all odd	u+v+w even	*X* odd	*n* = *X*	
		X even	*n* = *X*/2	
h, *k*, *l* all odd	u+v+w even	*X*/2 odd	*n* = *X*/2	
		X/2 even	*n* = *X*/4	

When the twin operation is a rotation of higher degree about [*uvw*], in general the rotational symmetry of the two-dimensional mesh in the (*hkl*) plane does no longer coincide with that of the twin operation. The degree of restoration of lattice nodes must now take into account the two-dimensional coincidence index Ξ for a plane of the family (*hkl*), which defines a super mesh in the twin lattice. Moreover, such a super mesh may exist in ξ planes out of N, depending on where is located the intersection of the [*uvw*] twin axis with the plane. The twin index n is finally given by:

$n = N\Xi/\xi$

9.24: Twin lattice

A twin operation overlaps both the direct and reciprocal lattices of the individuals that form a twin; consequently, the nodes of the individual lattices are overlapped (restored) to some extent. The (sub)lattice that is formed by the (quasi)restored nodes is the *twin lattice*. In case of non-zero twin obliquity the twin lattice suffers a slight deviation at the composition surface.

Let $H^* = \cap_i H_i$ be the intersection group of the individuals in their respective orientations, D(H*) the holohedral supergroup (proper or trivial) of H*, $D(\mathbf{L}_T)$ the point group of the twin lattice and $D(\mathbf{L}_{ind})$ the point group of the individual lattice. $D(\mathbf{L}_T)$ either coincides with D(H*) (case of zero twin obliquity) or is a proper supergroup of it (case of non-zero twin obliquity): it can be higher, equal or lower than $D(\mathbf{L}_{ind})$.

- When $D(\mathbf{L}_T) = D(\mathbf{L}_{ind})$ and the two lattices have the same orientation, twinning is by merohedry (twin index = 1). When at least some of the symmetry elements of $D(\mathbf{L}_T)$ are differently oriented from the corresponding ones of $D(\mathbf{L}_{ind})$, twinning is by reticular polyholohedry (twin index > 1, twin obliquity = 0) or reticular pseudopolyholohedry (twin index > 1, twin obliquity > 0).
- When $D(\mathbf{L}_T) \neq D(\mathbf{L}_{ind})$ twinning is by pseudomerohedry (twin index = 1, twin obliquity > 0),reticular merohedry (twin index > 1, twin obliquity = 0) or reticular pseudomerohedry (twin index > 1, twin obliquity > 0).

9.25: Twin law

The **twin law** is the set of twin operations mapping two individuals of a twin. It is obtained by coset decomposition of the point group of the twin lattice with respect to the intersection group of the point groups of the individuals in their respective orientations. Each operation in the same coset is a possible twin operation that, from the lattice viewpoint, is equivalent to any other operation in the same coset. Any of these can be taken as **coset representative** and indicated by the symbol of the twin element: $\bar{1}$, [*uvw*] and (*hkl*) for the centre (*inversion twin*), direction of the rotation axis (*rotation twin*) and Miller indices of the mirror plane (*reflection twin*), in the order. Except when one refers to a specific plane or direction, the symbols {*hkl*} or <*uvw*> have to be be used to indicate all the planes or directions which belong to the same coset and are therefore equivalent under the point group of the individual.

In case of TLQS twinning the equivalence of the operations in a coset is only approximate.

9.26: Twin obliquity

The concept of obliquity was introduced by Friedel in 1920 as a measure of the overlap of the lattices on the individuals forming a twin.

Let us indicate with $[u'v'w']$ the direction exactly perpendicular to a twin plane (hkl), and with $(h'k'l')$ the plane perpendicular to a twin axis [uvw]. $[u'v'w']$ is parallel to the reciprocal lattice vector $[hkl]^*$ and $(h'k'l')$ is parallel to the reciprocal lattice plane $(uvw)^*$. The angle between $[uvw]$ and $[u'v'w']$ or, which is the same, between (hkl) and $(h'k'l')$, is called the **obliquity ω**.

The vector in direct space $[uvw]$ has length $\mathrm{L}(uvw)$; the reciprocal lattice vector $[hkl]^*$ has length $\mathrm{L}^*(hkl)$. The obliquity ω is thus the angle between the vectors $[uvw]$ and $[hkl]^*$; the scalar product between these two vectors is

$\mathrm{L}(uvw)\ \mathrm{L}^*(hkl)\cos\omega = \langle uvw|hkl\rangle = uh + vk + wl$

where <| stands for a 1x3 row matrix and |> for a 3x1 column matrix.

It follows that

$\cos\omega = (uh + vk + wl)/\mathrm{L}(uvw)\mathrm{L}^*(hkl)$

where $\mathrm{L}(uvw) = \langle uvw|\mathbf{G}|uvw\rangle^{1/2}$ and $\mathrm{L}^*(hkl) = \langle hkl|\mathbf{G}^*|hkl\rangle^{1/2}$, $\mathbf{G}$ and $\mathbf{G}^*$ being the metric tensors in direct and reciprocal space, respectively.

Notice that $\mathbf{G}^* = \mathbf{G}^{-1}$ (and thus $\mathbf{G} = \mathbf{G}^{*-1}$) and that the matrix representation of the metric tensor is symmetric and coincides thus with its transpose ($\mathbf{G} = \mathbf{G}^{\mathrm{T}}$, $\mathbf{G}^* = \mathbf{G}^{*\mathrm{T}}$).

9.27: Twin operation

The operation (action) of an element of symmetry that generates a *twin*.

Let H_i be the oriented point group of the i-th individual of a twin. The intersection group of the oriented vector point groups H_i of the individuals is indicated as $H^* = \cap_i H_i$. The symmetry of a twin is identified in vector space by a point group K which is a supergroup of H*. The coset decomposition of K with respect to H* gives the possible twin laws, each coset representing a twin law, and each operation in a coset representing a twin operation; the operations in a coset are equivalent under the operations of H*.

Operations in H describe the vector point symmetry of the individuals, whereas those in the cosets obtained by decomposing K in terms of H* connect the different individuals. To underline their different nature, the twin operations are often associated with a "color" and K is a thus a chromatic vector point group, known as *twin point group*.

CHAPTER OVERVIEW

10: Biological Crystallography

Topic hierarchy

Contributors

10.1: Difference Patterson map

An application of Patterson methods for solution of crystal structures, typically proteins with heavy-atom derivatives, where the Patterson function is calculated using structure-factor coefficients based on the difference between the heavy-atom derivative and the native molecule.

10.2: Isomorphous replacement

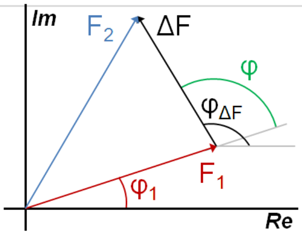


Figure: Principle of the isomorphous replacement method for structure solution. F_1 and F_2 represent the total structure factor from two isomorphous crystals for a given reflection, ΔF is their difference. The angles φ_1 and $\varphi_{\Delta F}$ are the phases of F_1 and ΔF, they are related via φ.

10.3: Maximum likelihood

An approach to structure refinement in which the parameters of a structural model are modified to optimize the statistical probability of generating a set of observed intensities. The technique is often used in the refinement of structures of biological macromolecules, where the unfavorable parameter-to-observation ratio often leads to overfitted data and consequent systematic errors in least-squares minimization procedures.

Contributors

10.4: Molecular Replacement

An approach to solving the phase problem by concentrating on phase relationships that arise through X-ray diffraction from similar molecular components. The components can be molecular fragments related through noncrystallographic symmetry (*e.g.* icosahedral subunits of a virus) or a similar molecule such as a homologous protein with high sequence identity.

Discussion

The technique is most commonly used in biological crystallography. Typically, an attempt is made to fit the structure under investigation (the 'target' structure) to a previously solved ('probe') structure. The probe may be a different crystal form of the same protein; or it may be a different protein with a high level of sequence identity, which correlates well with structural resemblance. As a rule of thumb, molecular replacement is often straightforward if the probe is well characterized and shares at least 40% sequence identity with the target. Rotation and transformation matrices must be applied. Patterson methods are suitable for determining the rotation function **R**, since intramolecular vectors are all shifted to the origin of a Patterson map. The orientational fit (*i.e.* the quality of the calculated rotation function) has usually been assessed by monitoring *R* factors or real-space correlation coefficients. Increasingly, modern programs use maximum likelihood based algorithms.

The translation function **T** is then determined to shift the now correctly orientated probe model to the correct coordinates within the asymmetric unit. Space-group symmetries can be used to help reduce the computationally intense calculations required.

History

Early applications of the technique concentrated on large virus structures with icosahedral symmetry. In the 1960s the early development of the molecular replacement technique was aimed primarily at *ab initio* phase determination. It was only in the 1970s, when more structures became available, that it was possible to use the technique to solve homologous structures with suitable search models .

See also

1. Noncrystallographic symmetry. D. M. Blow. *International Tables for Crystallography* (2006). Vol. F, ch. 13.1, pp. 263-268
2. Rossmann, M. G. & Blow, D. M. (1962). Acta Cryst. 15, 24–31. *The detection of sub-units within the crystallographic asymmetric unit.*

Contributors

10.5: Multiwavelength anomalous diffraction (MAD)

An approach to solving the phase problem in protein structure determination by comparing structure factors collected at different wavelengths, including the absorption edge of a heavy-atom scatterer. Also known as **multiple-wavelength anomalous diffraction** or **multiwavelength anomalous dispersion**.

Discussion

The 'normal' atomic scattering factor f^0 describes the strength of X-rays scattered from the electrons in an atom assuming that they are free oscillators. Because the scattering electrons are in fact bound in atomic orbitals, they act instead as a set of damped oscillators with resonant frequencies matched to the absorption frequencies of the electron shells. The total atomic scattering factor f is then a complex number, and is represented by the sum of the normal factor and real and imaginary 'anomalous' components:

$$f = f^0 + f' + i f''.$$

A consequence of the wavelength dependence of anomalous dispersion is that the structure factors will be significantly perturbed, both in amplitude and in phase, by resonant scattering off an absorption edge. Hence, if diffraction is carried out at a wavelength matching the absorption edge of a scattering atom, and again at a wavelength away from the absorption edge, comparison of the resulting diffraction patterns will allow information to be extracted about the phase differences. For suitable species, the effect is of comparing a native molecule with a strictly isomorphous derivative (and in such cases phase determination and improvement are similar to isomorphous replacement methods).

The technique, often using tunable synchrotron radiation, is particularly well suited to proteins where methionine residues can be readily replaced by selenomethionine derivatives; selenium has a sufficiently strong anomalous scattering effect that it allows phasing of a macromolecule.

History

This technique was introduced by W. Hendrickson (Hendrickson, W. A., 1991, *Determination of macromolecular structures from anomalous diffraction of synchrotron radiation*. *Science*, **254**, 51–58.)

See also

MAD and MIR. J. L. Smith, W. A. Hendrickson, T. C. Terwilliger and J. Berendzen. *International Tables for Crystallography* (2006). Vol. F, ch. 14.2, pp. 299-309

Contributors

10.6: Noncrystallographic symmetry

A symmetry operation that is not compatible with the periodicity of a crystal pattern (in two or three dimensions) is called a **noncrystallographic symmetry**. Rotations other than 1, 2, 3, 4, and 6 (in E^2 and E^3) belong to this type of symmetry. Rotations 5, 8, 10 and 12 are compatible with a translation in higher-dimensional spaces, but they are commonly considered noncrystallographic. For example、 in quasicrystals fivefold or tenfold rotational axes are incapable of tiling space through the application of three-dimensional lattice translations, but they act as normal symmetry axes in a higher-dimensional space. Continuous rotations, which give rise to the Curie groups contained in the cylindrical system and in the spherical system, are noncrystallographic in any dimension.

10.7: Optical resolution

By analogy with optical observations, *e.g.* in astronomy, the term **optical resolution** in structure determination,d_{opt}, is used to describe the expected minimum distance between two resolved peaks in an electron-density map.

$$d_{opt} = [2(\sigma^2_{Patt} + \sigma^2_{sph})]^{\frac{1}{2}}$$

where σ_{Patt} is the standard deviation of the Gaussian function fitted to the Patterson origin peak, σ_{sph} is the standard deviation of the Gaussian function fitted to the origin peak of the spherical interference function, representing the Fourier transform of a sphere with radius 1 / d_{min}, and d_{min} is the nominal resolution.

10.8: Real-space correlation coefficient

The real-space correlation coefficient, RSCC, is a measure of the similarity between an electron-density map calculated directly from a structural model and one calculated from experimental data. An advantage of techniques for evaluating goodness of fit in real space is that they can be performed for arbitrary sets of atoms. They are therefore used most often in the refinement of biological macromolecular structures to improve the model fit on a per-residue basis.

$$\mathrm{RSCC} = \frac{\sum |\rho_{obs} - \langle \rho_{obs} \rangle| \sum |\rho_{calc} - \langle \rho_{calc} \rangle|}{\sqrt{\sum |\rho_{obs} - \langle \rho_{obs} \rangle|^2 \sum |\rho_{calc} - \langle \rho_{calc} \rangle|^2}}$$

(ρ's are electron density values at grid points that cover the residue in question, obs and calc refer to experimental and model electron density, respectively.)

This metric is similar to the real-space residual RSR, but does not require that the two densities be scaled against each other.

10.9: Real-space residual

The real-space residual, RSR, is a measure of the similarity between an electron-density map calculated directly from a structural model and one calculated from experimental data. An advantage of techniques for evaluating goodness of fit in real space is that they can be performed for arbitrary sets of atoms. They are therefore used most often in the refinement of biological macromolecular structures to improve the model fit on a per-residue basis.

$$\text{RSR} = \frac{\sum |\rho_{obs} - \rho_{calc}|}{\sum |\rho_{obs} + \rho_{calc}|}$$

(ρ's are electron density values at grid points that cover the residue in question, obs and calc refer to experimental and model electron density, respectively.)

The measure of similarity is often provided in the form of a graph of RSR values against residue number, showing clearly which residues give best and worst agreement with the experimental electron-density map. For nucleic acid structures, RSR may also be calculated separately for base, sugar and phosphate moieties of the nucleic acid monomer. RSR is generally considered an excellent model-validation tool.

10.10: Sohncke groups

Sohncke groups are called the 65 three-dimensional space groups containing only operations of the first kind (rotations, rototranslations, translations). It is very generally accepted that enantiomerically-pure compounds (e.g. proteins) crystallize in these groups. The term comes from Leonhard Sohncke (Halle, 22 February 1842 – München, 1 November 1897), German mathematician.

Contributors

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Sample Word 1 | Sample Definition 1

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