Crystal Structures and Symmetries

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B 1 Crystal Structures and Symmetries

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Introduction

The term "crystal" derives from the Greek κρύσταλλος , which was first used as description of ice and later - in a more general meaning - for transparent minerals with regular morphology (regular crystal faces and edges).

Crystalline solids are thermodynamically stable in contrast to amorphous solids and are characterised by a **regular three-dimensional periodic arrangement of atoms** (ions, molecules) in space. This periodic arrangement makes it possible to determine their structure (atomic positions in 3D space) by **diffraction methods**, using the crystal lattice as a three-dimensional diffraction grating.

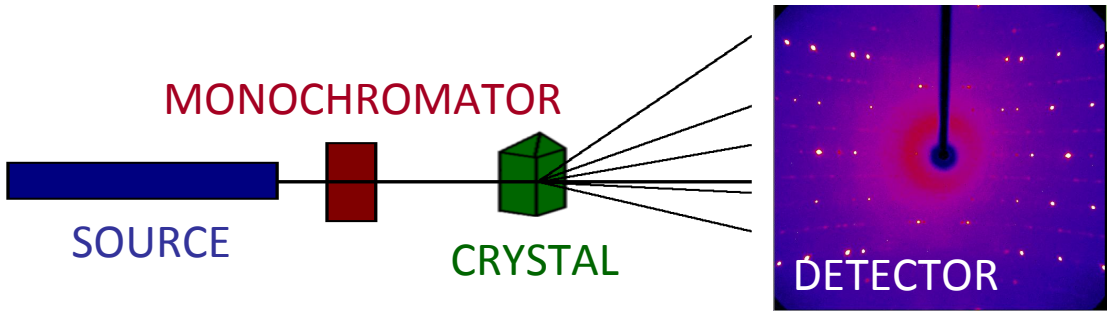


Fig. 1.1: *Sketch of a typical constant wavelength single crystal diffraction experiment. The first such experiment has been conducted by Laue et al. in 1912 (Nobel Prize in Physics 1914).*

The purpose of this chapter is to give a brief introduction into the symmetry concept underlying the description of the crystalline state.

1.1 Crystal lattices

The three-dimensional periodicity of crystals can be represented by the so-called crystal lattice. The repeat unit in form of a parallelepiped - known as the **unit cell** – is defined by 3 non-coplanar basis vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, and $\boldsymbol{a}_3$, whose directions form the reference axes of the corresponding right-handed crystallographic coordinate system. The 6 **lattice parameters** are given as the lengths of the basis vectors $a = |\boldsymbol{a}_1|$, $b = |\boldsymbol{a}_2|$, $c = |\boldsymbol{a}_3|$ and the angles between the basis vectors: angle $(\boldsymbol{a}_1,\boldsymbol{a}_2) = \gamma$, angle $(\boldsymbol{a}_2,\boldsymbol{a}_3) = \alpha$, angle $(\boldsymbol{a}_3,\boldsymbol{a}_1) = \beta$. The faces of the unit cell are named as face $(\boldsymbol{a}_1,\boldsymbol{a}_2)$ = C**,** face $(\boldsymbol{a}_2,\boldsymbol{a}_3)$ = A**,** face $(\boldsymbol{a}_3,\boldsymbol{a}_1)$ = B.

If the vertices of all repeat units (unit cells) are replaced by points, the result is the crystal lattice in the form of a **point lattice**. Each lattice point is given by a vector $\boldsymbol{a} = u\boldsymbol{a}_1+v\boldsymbol{a}_2+w\boldsymbol{a}_3$, with u, v, w being integers. As a symmetry operation of parallel displacement, $\boldsymbol{a}$ – also known as **translation vector** – maps the atomic arrangement of the crystal (crystal structure) onto itself.

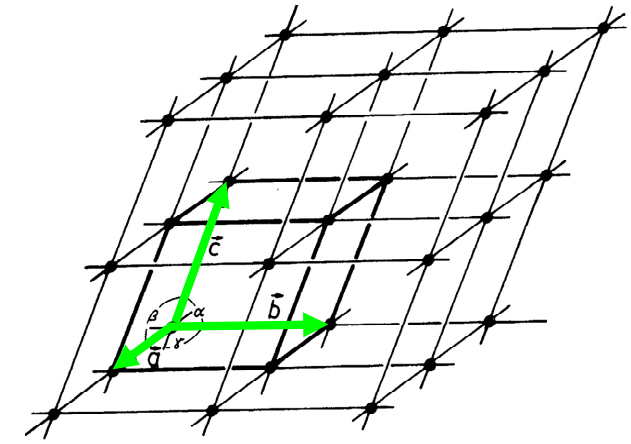


Fig. 1.2: *Notation for a unit cell (basis vectors* $\boldsymbol{a_1}$, $\boldsymbol{a_2}$, $\boldsymbol{a_3}$, *or a, b, c) and a point lattice.*

A **lattice point** is labelled "*uvw*", according to the coefficients (integers) of the translation vector

$$\boldsymbol{a} = u\,\boldsymbol{a_1} + v\,\boldsymbol{a_2} + w\,\boldsymbol{a_3} \qquad 1.1$$

from the origin to the lattice point. A **lattice direction** - given by the symbol [*uvw*] - is defined by the direction of the corresponding translation vector.

A plane passing through three lattice points is known as a **lattice plane**. Since all lattice points are equivalent (by translation symmetry) there will be infinitely many parallel planes passing through all the other points of the lattice. Such a set of equally spaced planes is known as a **set of lattice planes**. If the first plane from the origin of a set of lattice planes makes intercepts a_1/h, a_2/k, a_3/l on the axes, where h, k, l are integers, then the **Miller indices** of this set of lattice planes are (hkl), the three coefficients h, k, l are conventionally enclosed in parentheses.

The equation of lattice planes can be written in intercept form as

$$(h\mathrm{x}/a_1) + (k\mathrm{y}/a_2) + (l\mathrm{z}/a_3) = \mathrm{n}, \qquad 1.2$$

where n is an integer. If n = 0 the lattice plane passes through the origin; if n = 1 the plane makes intercepts a_1/h, a_2/k, a_3/l on the axes; if n = 2 the intercepts are $2a_1/h$, $2a_2/k$, $2a_3/l$; and so on.

Complementary to the crystal lattice, the so-called reciprocal lattice may be constructed, which is a useful tool for understanding the geometry of diffraction experiments. The reciprocal lattice can be thought of as the result of diffraction (of X-rays, neutrons, electrons etc.) from the crystal lattice ('direct lattice'). The points on the diffraction pattern in Fig. 1.1 (right) are actually points of the reciprocal lattice recorded during the diffraction experiment. Their nodes are indexed by the Miller-indices hkl in the same way as the nodes of the direct lattice are indexed by uvw:

$$\boldsymbol{\tau} = h\,\boldsymbol{\tau_1} + k\,\boldsymbol{\tau_2} + l\,\boldsymbol{\tau_3}. \qquad 1.3$$

The basis vectors $\boldsymbol{\tau}$ of the reciprocal lattice can be calculated from those of the direct cell by:

$$\boldsymbol{\tau}_i = (\mathbf{a}_j \times \mathbf{a}_k)/V_c, \qquad 1.4$$

where × means the cross product, and $V_c = \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)$ is the volume of the unit cell.

Here is a compilation of some properties of the reciprocal lattice:

- Each reciprocal lattice vector is perpendicular to two real space vectors: $\boldsymbol{\tau}_i \perp \mathbf{a}_j$ and $\mathbf{a}_k$ (for $i \neq j, k$)
- The lengths of the reciprocal lattice vectors are $|\boldsymbol{\tau}_i| = 1/V_c \cdot |\mathbf{a}_j| \cdot |\mathbf{a}_k| \cdot \sin\angle(\mathbf{a}_j, \mathbf{a}_k)$.
- Each point *hkl* in the reciprocal lattice refers to a set of planes (*hkl*) in real space.
- The direction of the reciprocal lattice vector $\boldsymbol{\tau}$ is normal to the (*hkl*) planes and its length is reciprocal to the interplanar spacing d_{hkl}: $|\boldsymbol{\tau}| = 1/d_{hkl}$.
- Duality principle: The reciprocal lattice of the reciprocal lattice is the direct lattice.

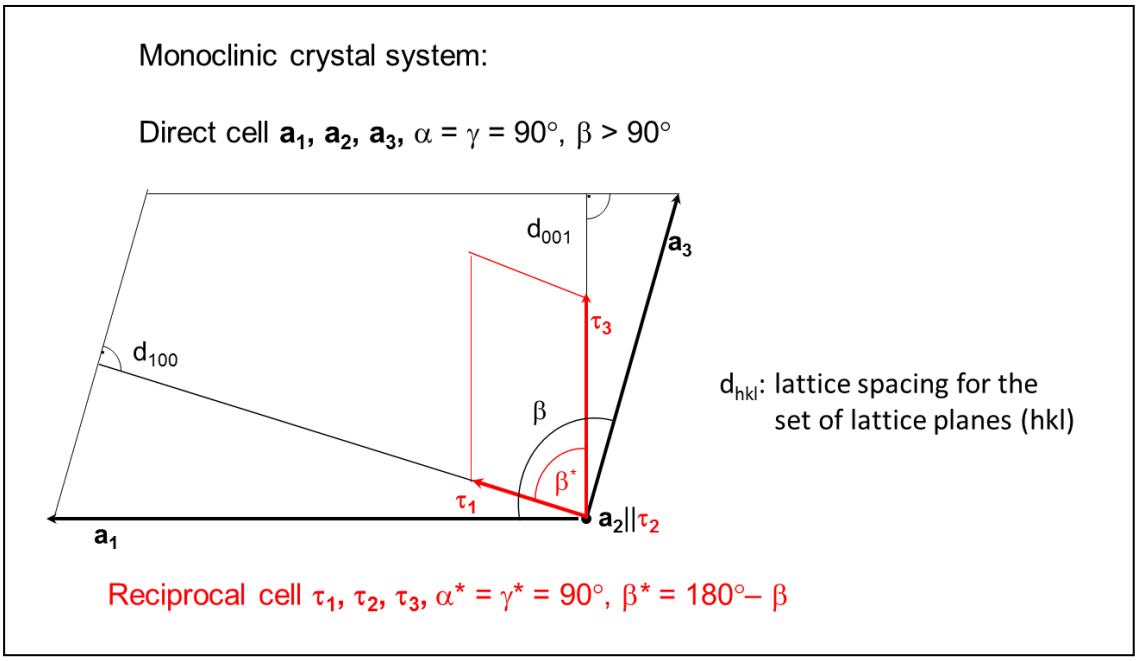


Fig. 1.3: Direct and corresponding reciprocal unit cell.

1.2 Crystallographic coordinate systems

The description of a crystal structure consists first of the choice of a unit cell as the smallest repeat unit of the crystal with its basis vectors. In this way a crystal-specific coordinate system is defined which is used to localize all the atoms in the unit cell. While - in physics and chemistry - Cartesian coordinate systems are frequently used, crystallographers often use non-orthogonal and non-orthonormal coordinate systems.

The conventional crystallographic coordinate systems are based on the symmetry of the crystals. In three dimensions there are **7** different **crystal systems** and hence 7 crystallographic coordinate systems:

Crystal system	Minimum symmetry	Conventional unit cell
triclinic	1 or $\bar{1}$	$a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$
monoclinic (unique axis b)	one diad – 2 or m ($\parallel Y$)	$a \neq b \neq c$; $\alpha=\gamma=90°$, $\beta>90°$
orthorhombic	three mutually perpendicular diads – 2 or m ($\parallel X$, Y and Z)	$a \neq b \neq c$; $\alpha=\beta=\gamma=90°$
tetragonal	one tetrad – 4 or $\bar{4}$ ($\parallel Z$)	$a = b \neq c$; $\alpha=\beta=\gamma=90°$
trigonal (hexagonal cell)	one triad – 3 or $\bar{3}$ ($\parallel Z$)	$a = b \neq c$; $\alpha=\beta=90°$, $\gamma=120°$
hexagonal	one hexad – 6 or $\bar{6}$ ($\parallel Z$)	$a = b \neq c$; $\alpha=\beta=90°$, $\gamma=120°$
cubic	four triads – 3 or $\bar{3}$ ($\parallel$space diagonals of cube)	$a = b = c$; $\alpha=\beta=\gamma=90°$

The choice of the origin of the coordinate system is free in principle, but for convenience it is usually chosen at a centre of symmetry (inversion centre), if present, otherwise in a point of high symmetry.

In order to complete the symmetry conventions of the coordinate systems it is necessary to add to the 7 so-called primitive unit cells of the crystal systems (primitive lattice types with only one lattice point per unit cell) 7 centred unit cells with two, three or four lattice points per unit cell (centred lattice types). These centred unit cells are consequently two, three or four times larger than the smallest repeat units of the crystals. The resulting **14 Bravais lattice types** with their centering conditions are collected in Fig. 1.4.

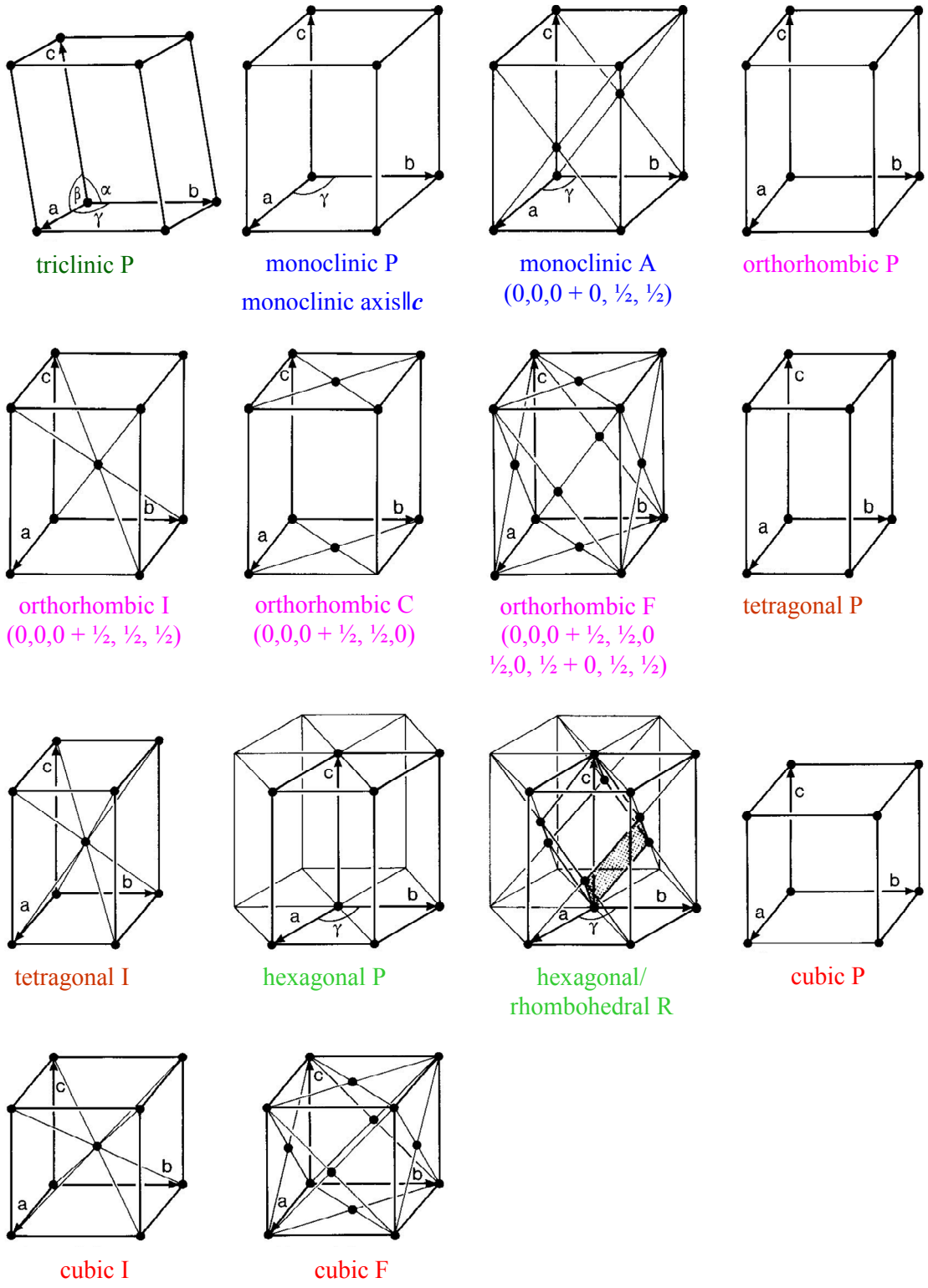


Fig. 1.4: *The 14 Bravais lattices consisting of the 7 primitive lattices P for the 7 crystal systems with only one lattice point per unit cell + the 7 centred (multiple) lattices A, B, C, I, R and F with 2, 3 and 4 lattice points per unit cell.*

1.3 Symmetry-operations and -elements

The **symmetry operations** of a crystal are isometric transformations or motions, i.e. mappings which preserve distances and, hence, also angles and volumes. An object and its transformed object superimpose in a perfect manner, they are indistinguishable.

The simplest crystallographic symmetry operation is the **translation**, which is a parallel displacement of the crystal by a translation vector $\boldsymbol{a}$ (see chapter 1.1). There is no fixed point, the entire lattice is shifted and therefore, theoretically, the crystal lattice is considered to be infinite.

Crystallographic **rotations** n around an axis by an angle $\varphi = 360°/n$ (n-fold rotations) and **rotoinversions** (combination of rotations and inversions) $\bar{n}$ are called point symmetry operations because they leave at least one point of space invariant (at least one fixed point). An important fact of crystallographic symmetry is the restriction of the rotation angles by the three-dimensional crystal lattice to $\varphi = 360°$ (n = 1), 180° (n = 2), 120° (n = 3), 90° (n = 4), 60° (n = 6). Only for these crystallographic rotations the space can be covered completely without gaps and overlaps. The rotoinversion $\bar{n} = \bar{1}$ is an **inversion** in a point, $\bar{n} = \bar{2} \equiv m$ (mirror) describes a **reflection** across a plane.

The combination of n-fold rotations with $(m/n)\cdot\boldsymbol{a}$ translation components (m < n) ∥ to the rotation axis leads to the so-called **screw rotations** n_m, e.g. 2_1, 3_2, 4_2, 6_5. These symmetry operations have no fixed points.

The combination of a reflection through a plane (glide plane) with translation components (glide vectors) of $\boldsymbol{a_1}/2$, $\boldsymbol{a_2}/2$, $\boldsymbol{a_3}/2$, $(\boldsymbol{a_1}+\boldsymbol{a_2})/2$, … ∥ to this plane are known as **glide reflections** a, b, c, n, …, d. Again no fixed points exist for these symmetry operations.

In addition to the symmetry operations which represent isometric motions of an object, symmetry can also be described in (static) geometrical terms by **symmetry elements**. They form the geometrical locus, oriented in space, on which a symmetry operation is performed (line for a rotation, plane for a reflection, and point for an inversion) together with a description of this operation. Symmetry elements are mirror planes, glide planes, rotation axes, screw axes, rotoinversion axes and inversion centres. The geometrical descriptions of the crystallographic symmetry operations are illustrated in Figs. 1.5-1.7.

A symmetry operation transforms a point X with coordinates x, y, z (according to a position vector $\boldsymbol{X} = x\boldsymbol{a_1} + y\boldsymbol{a_2} + z\boldsymbol{a_3}$) into a symmetrically equivalent point X' with coordinates x', y', z' mathematically by the linear equations

$$\begin{aligned} x' &= W_{11}x + W_{12}y + W_{13}z + w_1 \\ y' &= W_{21}x + W_{22}y + W_{23}z + w_2 \\ z' &= W_{31}x + W_{32}y + W_{33}z + w_3 \end{aligned} \qquad 1.5$$

with w_1, w_2, w_3 constituting the translational part of the symmetry operation.

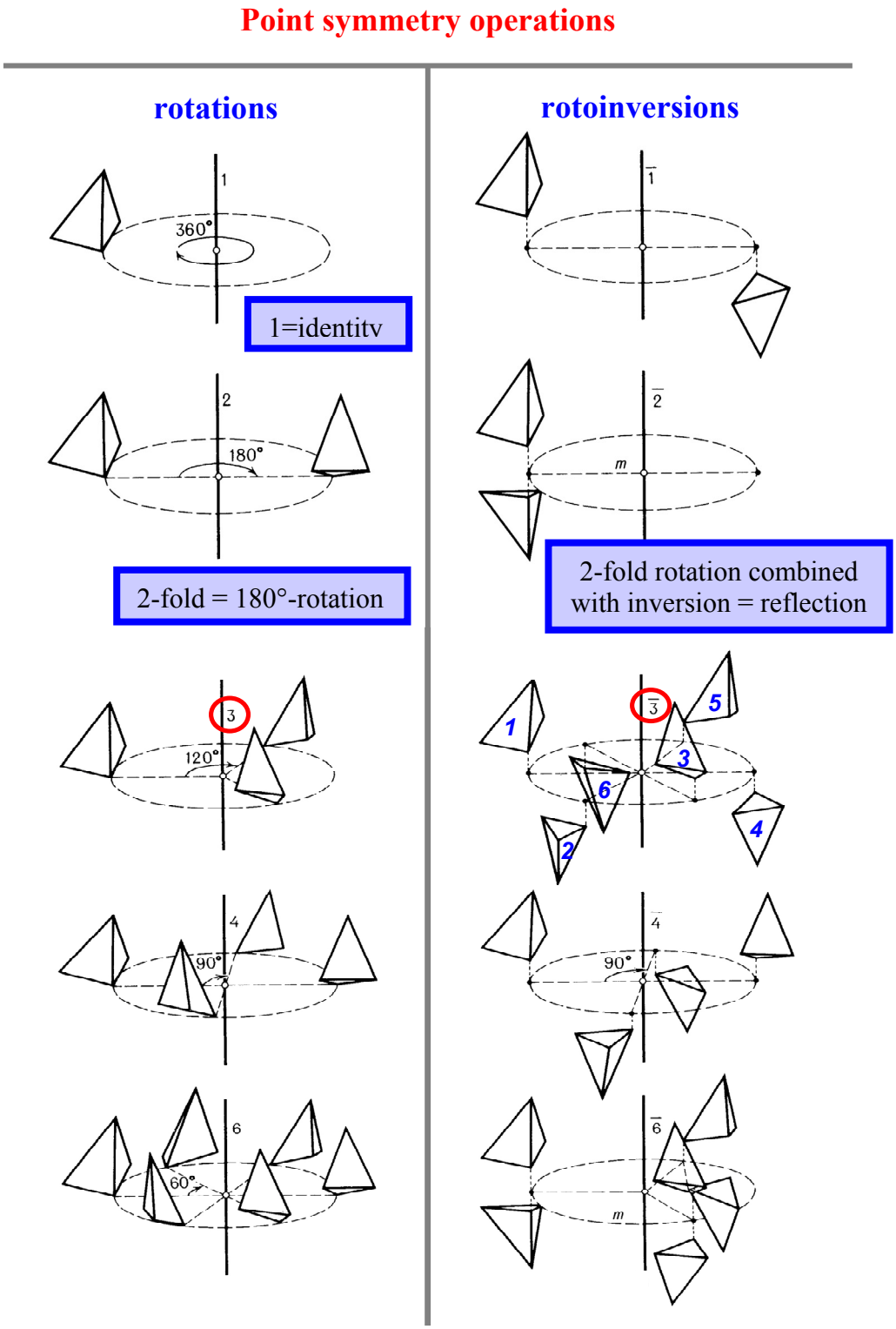


Fig. 1.5: *Rotations: n=1 (identity), n=2 (rot. angle 180°), n=3 (120°), n=4 (90°), n=6 (60°). Rotoinversions: $\bar{1}$ (inversion), $\bar{2} \equiv m$ (reflection), 3=3+1, $\bar{4}$, $\bar{6}$ = 3/m.*

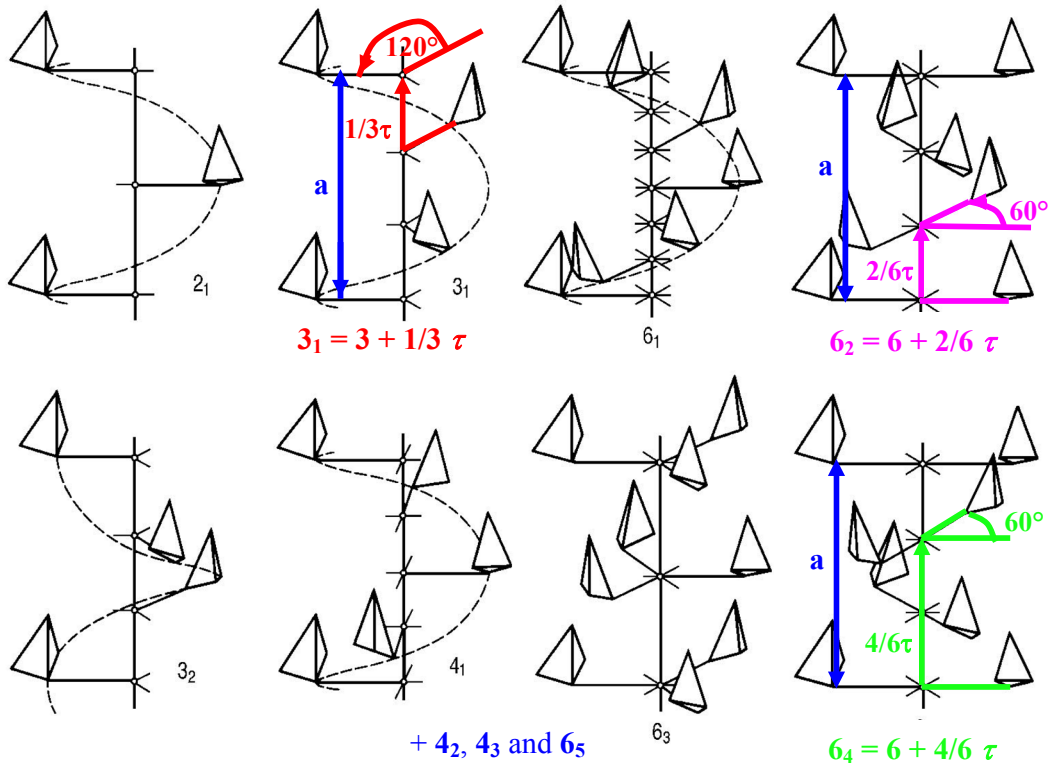


Fig. 1.6: *Screw rotations n_m: combination of rotations n and translation components (m/n)·a ∥ to the rotation axis.*

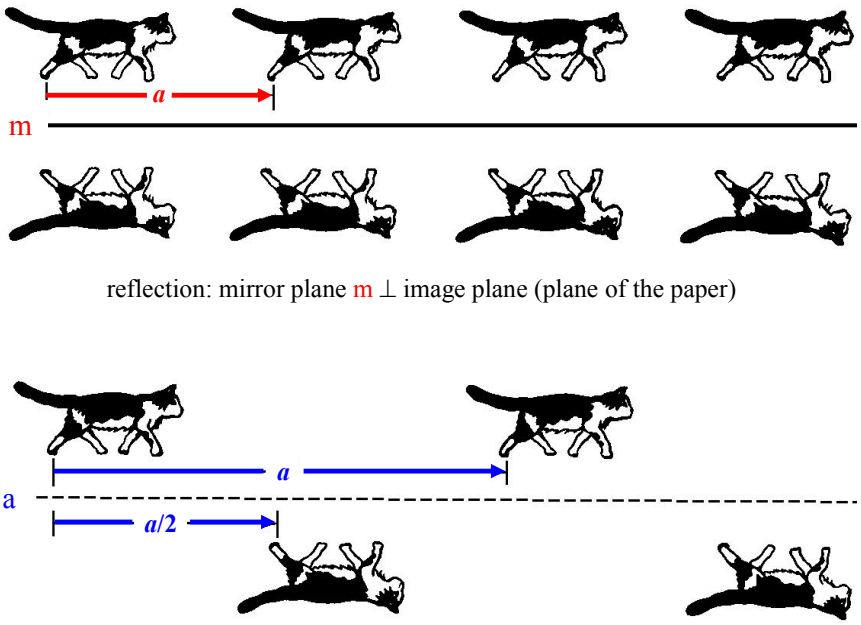


Fig. 1.7: *Examples of reflections and glide reflections.*

The above equation, re-written in matrix notation:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix} \circ \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}; \quad \boldsymbol{X}' = \mathbf{W} \circ \boldsymbol{X} + \boldsymbol{w} = (\mathbf{W}, \mathbf{w}) \circ \boldsymbol{X} \qquad 1.6$$

The (3×3) matrix **W** is the rotational part and the (3×1) column matrix ***w*** the translational part of the symmetry operation. The two parts **W** and ***w*** can be assembled into an augmented (4×4) matrix ***W*** according to

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \begin{pmatrix} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \circ \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = \boldsymbol{W} \circ \boldsymbol{X} \qquad 1.7$$

Since every symmetry transformation is a "rigid-body" motion, the determinant of all matrices **W** and ***W*** is det **W** = det ***W*** = ± 1 (+ 1: preservation of handedness; - 1: change of handedness of the object).

The sequence of two symmetry operations (successive application) is given by the product of their matrices $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$:

$$\boldsymbol{W_3} = \boldsymbol{W_1} \circ \boldsymbol{W_2} \qquad 1.8$$

where $\boldsymbol{W_3}$ is again a symmetry operation.

1.4 Crystallographic point groups and space groups

The symmetry of a crystal and of its crystal structure can be described by mathematical group theory. The symmetry operations are the group elements of a crystallographic group G and the combination of group elements is the successive execution of symmetry operations. All possible combinations of crystallographic point-symmetry operations in three-dimensional space lead to exactly 32 crystallographic point groups (≡ crystal classes) which all are of finite order (the maximum order is 48 for the cubic crystal class $m\bar{3}m$). For the different crystal systems they are represented by stereographic projections in Fig. 1.8. There are two types of group symbols in use: For each crystal class the corresponding Schoenflies symbol is given at the bottom left and the Hermann-Mauguin (international) symbol at the bottom right. A maximum of 3 independent main symmetry directions ("Blickrichtungen") is sufficient to describe the complete symmetry of a crystal. These symmetry directions are specifically defined for the 7 crystal systems (Hermann-Mauguin symbols). As an example, the symmetry directions of the cubic system are shown in Fig. 1.9.

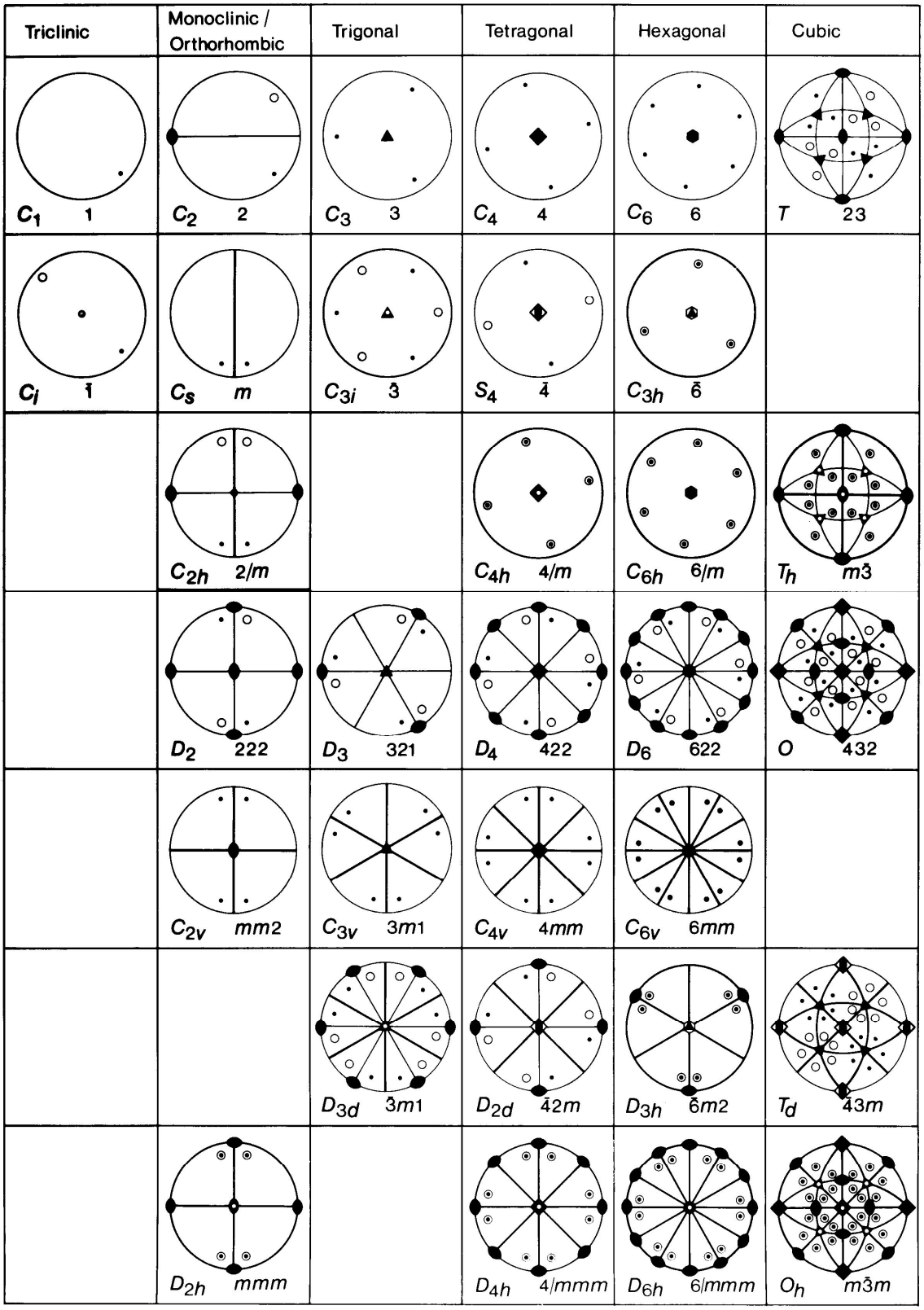


Fig. 1.8: *The 32 crystallographic point groups (crystal classes) in three-dimensional space represented by their stereographic projections. The group symbols are given according to Schoenflies (bottom left) and to Hermann-Mauguin (bottom right).*

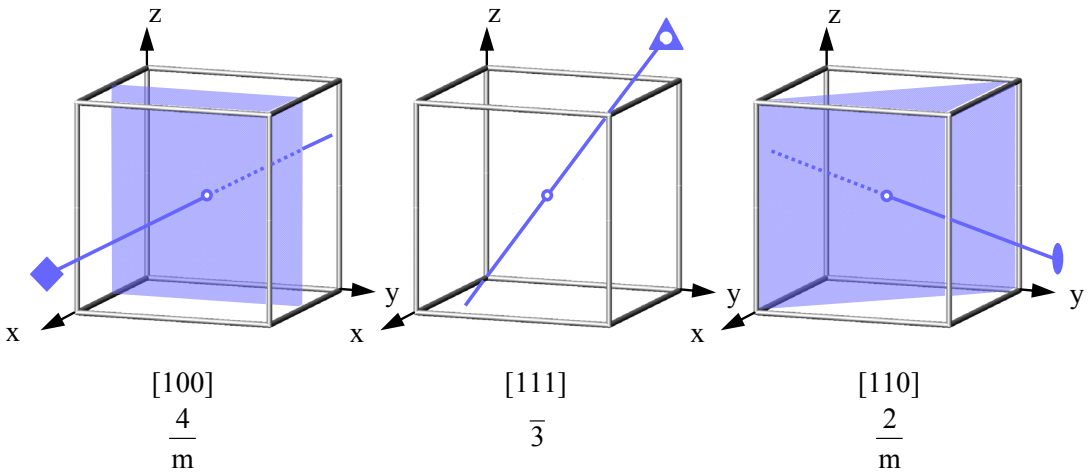


Fig. 1.9: *Symmetry directions ("Blickrichtungen") of the cubic lattice (a=b=c, α=β=γ=90°). Along [100]: 4/m, along [111]: $\bar{3}$, along [110]: 2/m.*

In three dimensions all possible combinations of the point symmetries of the 32 crystallographic point groups with the lattice translations of the 14 Bravais lattices lead to exactly 230 space groups, all of infinite order. As already mentioned, the addition of translations to the point symmetries results in new symmetry operations: Screw rotations and glide reflections. The conventional graphical symbols for the symmetry elements according to the International Tables for Crystallography Vol. A (2002) [1] are shown in Fig. 1.10.

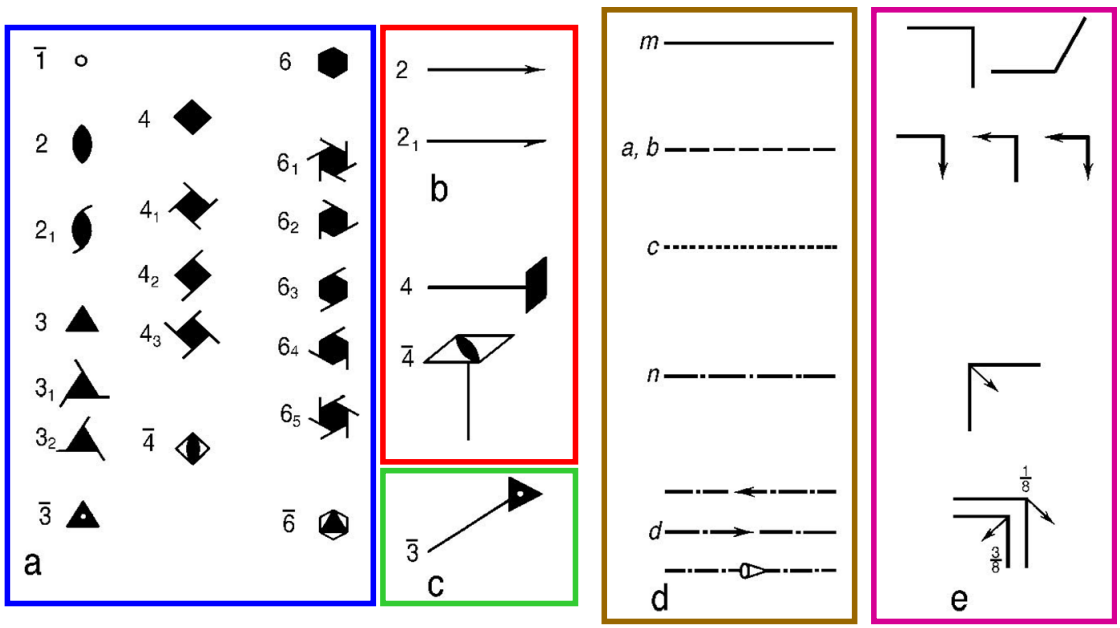


Fig. 1.10: *Conventional graphical symbols for symmetry elements:*
- symmetry axes: (a) perpendicular, (b) parallel, and (c) inclined to the plane;
- symmetry planes: (d) perpendicular and (e) parallel to the image plane.

1.5 Quasicrystals

Since the pioneering work of Shechtman et al [2] published in 1984 and honoured by the 2011 Nobel-Prize in Physics it is accepted that the crystalline state with its 3D periodic arrangement of atoms in a lattice is not the only long-range ordered ground state of matter. This quasi crystalline state also follows strict construction rules and exhibits long range order, but the rules are no longer based on the lattice concept.

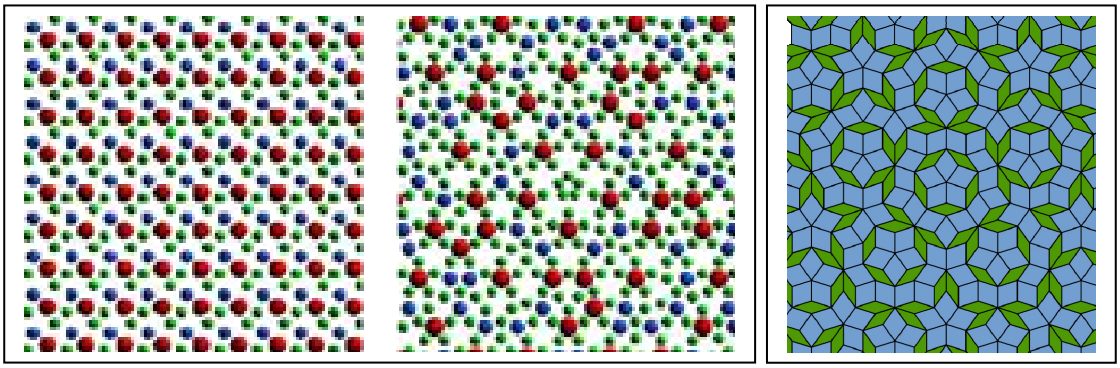


Fig. 1.11: 2D-analogues of a crystalline (left) and a quasi-crystalline structure (center) [3], Penrose tiling of a plane by two different rhombs (right) [4].

The description of quasicrystals is closely related to the so called Penrose-tilings which are a way to cover the plane completely and without overlap by a long range ordered, non-periodic arrangement of (in the case shown in Fig. 1.11) two different geometric shapes (here: rhombs). As a result of the lack of translation symmetry, the "crystallographically forbidden" rotation axes (5-fold, 8-fold, 10-fold etc., more precisely: forbidden as part of a 3D-space group symmetry) may occur in quasi crystals and also show up as symmetries of the outer shape (Fig. 1.12 left) and diffraction patterns of quasi crystals (center).

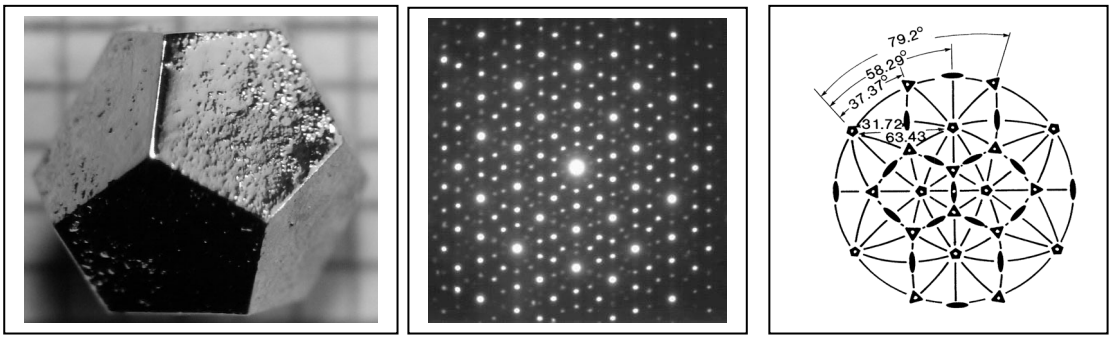


Fig. 1.12: Icosahedral quasi crystal HoMgZn (left) [5], electron diffraction pattern taken along the -5 rotoinversion axis (center) [5] and stereographic projection of the icosahedral point symmetry group m-3-5 [2]

1.6 Application: Structure description of $YBa_2Cu_3O_{7-\delta}$

The crystal structure determination with atomic resolution is achieved by diffraction experiments with X-rays, electron or neutron radiation. As an example, the results of a structure analysis by neutron diffraction on a single crystal of the ceramic high-T_C superconductor $YBa_2Cu_3O_{7-\delta}$ with T_C = 92 K are presented [6]. The atomic arrangement of the orthorhombic structure, space group P m m m, and the temperature-dependent electrical resistivity are shown in Fig. 1.13.

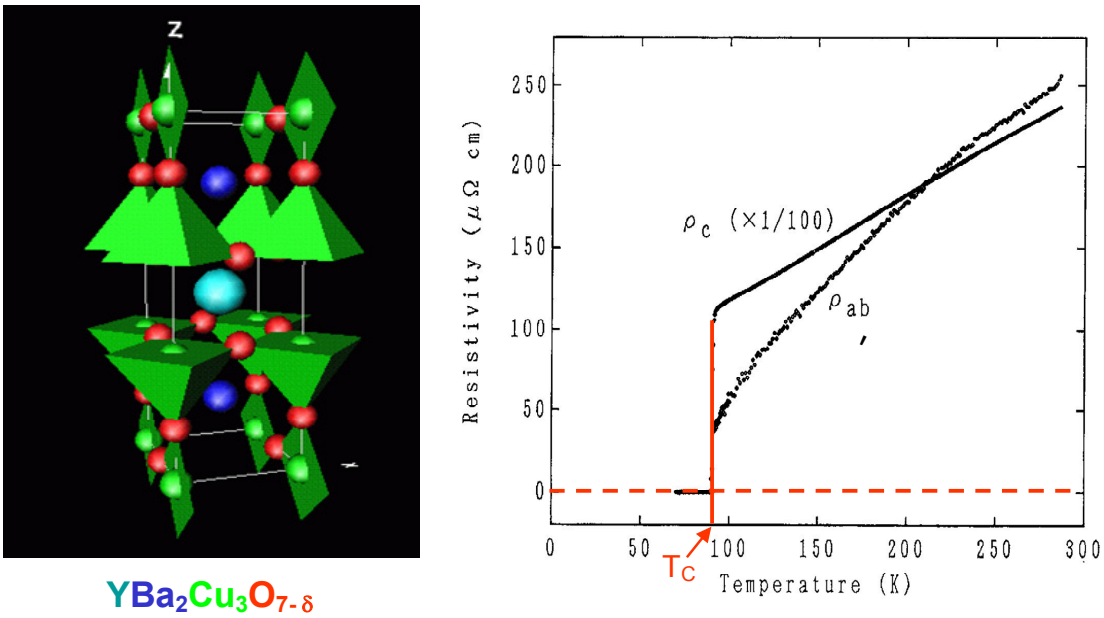
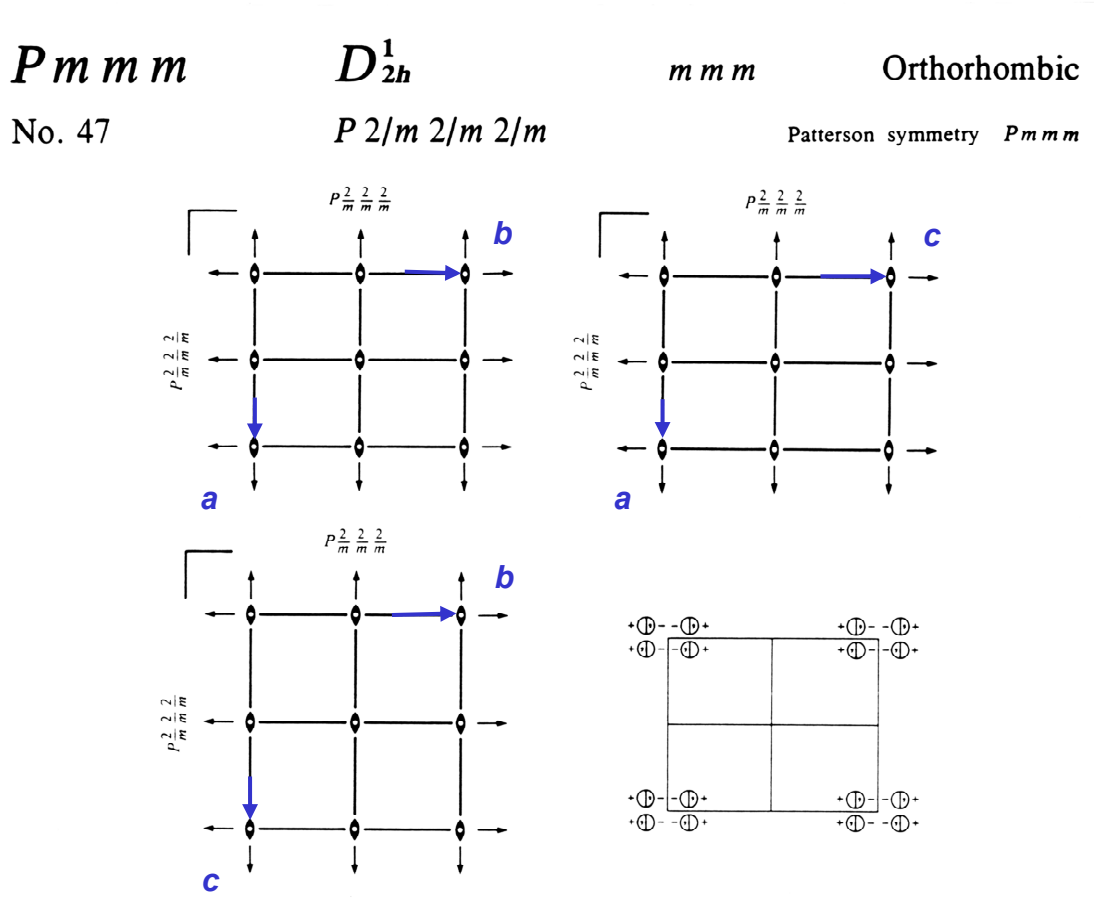


Fig. 1.13: *Crystal structure (unit cell) of $YBa_2Cu_3O_{7-\delta}$ with the CuO_x-polyhedra (left) and the electrical resistivity as a function of temperature ∥ and ⊥ to the [001] direction (right).*

The crystal structure contains two different Cu-O polyhedra (green): CuO_5-tetragonal pyramids and CuO_4-squares. The pyramids share corners in 2D and form double layers, the charge carriers responsible for superconductivity are supposed to be located in these double layers.

Information from the international tables on the relative locations and orientations of the symmetry elements (symmetry operations 1, 2_z, 2_y, 2_x, $\bar{1}$, m_z, m_y, m_x) of the orthorhombic space group P m m m, together with the choice of the origin (in an inversion centre), is shown in Fig. 1.14. The general position (site symmetry 1) of multiplicity 8 and all special positions with their site symmetries are listed in Fig. 1.15. There are no special reflection conditions for this space group.



Origin at centre ($m\,m\,m$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 0,0,z (3) 2 0,y,0 (4) 2 x,0,0
(5) $\bar{1}$ 0,0,0 (6) m x,y,0 (7) m x,0,z (8) m 0,y,z

Fig. 1.14: *Description of the orthorhombic space group P m m m in [1].*

CONTINUED $YBa_2Cu_3O_{7-\delta}$ No. 47 *Pmmm*

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	α	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$	no conditions
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z$	(8) $\bar{x},y,z$	
							Special: no extra conditions
4	z	$..m$	$x,y,\frac{1}{2}$	$\bar{x},\bar{y},\frac{1}{2}$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	
4	y	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,0$	$x,\bar{y},0$	
4	x	$.m.$	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$	$\bar{x},\frac{1}{2},\bar{z}$	$x,\frac{1}{2},\bar{z}$	
4	w	$.m.$	$x,0,z$	$\bar{x},0,z$	$\bar{x},0,\bar{z}$	$x,0,\bar{z}$	
4	v	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	
4	u	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	
2	t	$mm2$	$\frac{1}{2},\frac{1}{2},z$	$\frac{1}{2},\frac{1}{2},\bar{z}$			
2	s	$mm2$	$\frac{1}{2},0,z$	$\frac{1}{2},0,\bar{z}$			
2	r	$mm2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}$			
2	q	$mm2$	$0,0,z$	$0,0,\bar{z}$			
2	p	$m2m$	$\frac{1}{2},y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\frac{1}{2}$			
2	o	$m2m$	$\frac{1}{2},y,0$	$\frac{1}{2},\bar{y},0$			
2	n	$m2m$	$0,y,\frac{1}{2}$	$0,\bar{y},\frac{1}{2}$			
2	m	$m2m$	$0,y,0$	$0,\bar{y},0$			
2	l	$2mm$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$			
2	k	$2mm$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$			
2	j	$2mm$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$			
2	i	$2mm$	$x,0,0$	$\bar{x},0,0$			
1	h	mmm	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$				
1	g	mmm	$0,\frac{1}{2},\frac{1}{2}$				
1	f	mmm	$\frac{1}{2},\frac{1}{2},0$				
1	e	mmm	$0,\frac{1}{2},0$				
1	d	mmm	$\frac{1}{2},0,\frac{1}{2}$				
1	c	mmm	$0,0,\frac{1}{2}$				
1	b	mmm	$\frac{1}{2},0,0$				
1	a	mmm	$0,0,0$				

Fig. 1.15: *General and special positions (coordinates of all symmetrically equivalent positions) of space group P m m m with their site symmetries and multiplicities [1]. The special positions occupied by atoms of the $YBa_2Cu_3O_{7-\delta}$ structure are highlighted by frames.*

The atomic parameters of the structure refinement of $YBa_2Cu_3O_{6.96}$ at room temperature [6] are given in the following Table:

Atomic positions of $YBa_2Cu_3O_{6.96}$ orthorhombic, space group type P *2/m 2/m 2/m* *a* = 3.858 Å, *b* = 3.846 Å, *c* = 11.680 Å (at room temperature)					
atom/ion	**multiplicity**	**site symmetry**	**x**	**y**	**z**
$Cu1/Cu^{2+}$	1	*2/m 2/m 2/m*	0	0	0
$Cu2/Cu^{2+}$	2	*m m 2*	0	0	0.35513(4)
Y/Y^{3+}	1	*2/m 2/m 2/m*	½	½	½
Ba/Ba^{2+}	2	*m m 2*	½	½	0.18420(6)
$O1/O^{2-}$	2	*m m 2*	0	0	0.15863(5)
$O2/O^{2-}$	2	*m m 2*	0	½	0.37831(2)
$O3/O^{2-}$	2	*m m 2*	½	0	0.37631(2)
$O4/O^{2-}$	1	*2/m 2/m 2/m*	0	½	0

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