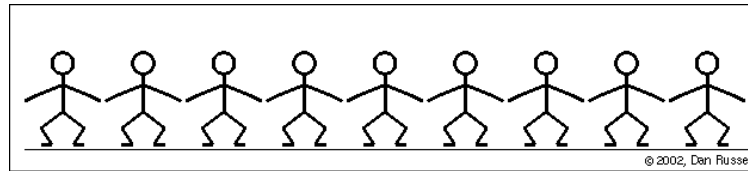
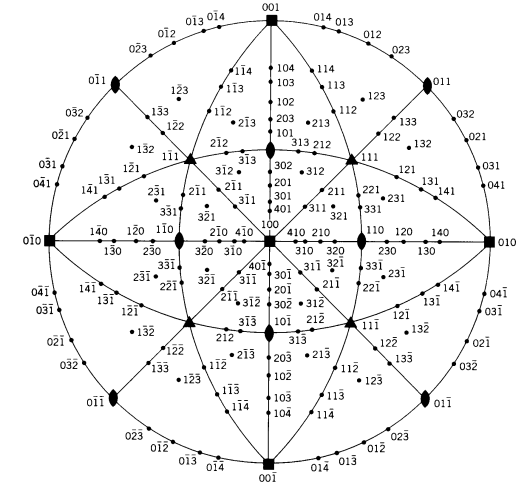


Crystallography Basics 2010



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Number of students falling a sleep



Basic Crystallography - Objectives

- Describe the position of atoms in a crystal
- Reduce this description to the most compact form using symmetry operations (Euclidean mapping – translations, rotations and reflections)
- Understand the structure of crystal
- Provide methods for calculating the distance between planes, repeat lengths along directions, angles between planes and directions and diffracting power

Plan

- Direct space – the real world
- Fractional coordinates
- Symmetry operations
- Lattice planes and directions
- Point groups
- Crystallographic calculations (structure factor, angles, d-space, reciprocal lattice, metric tensor and orthogonal basis)

230 Space Groups

The 230 three-dimensional space groups arranged by crystal systems and point groups

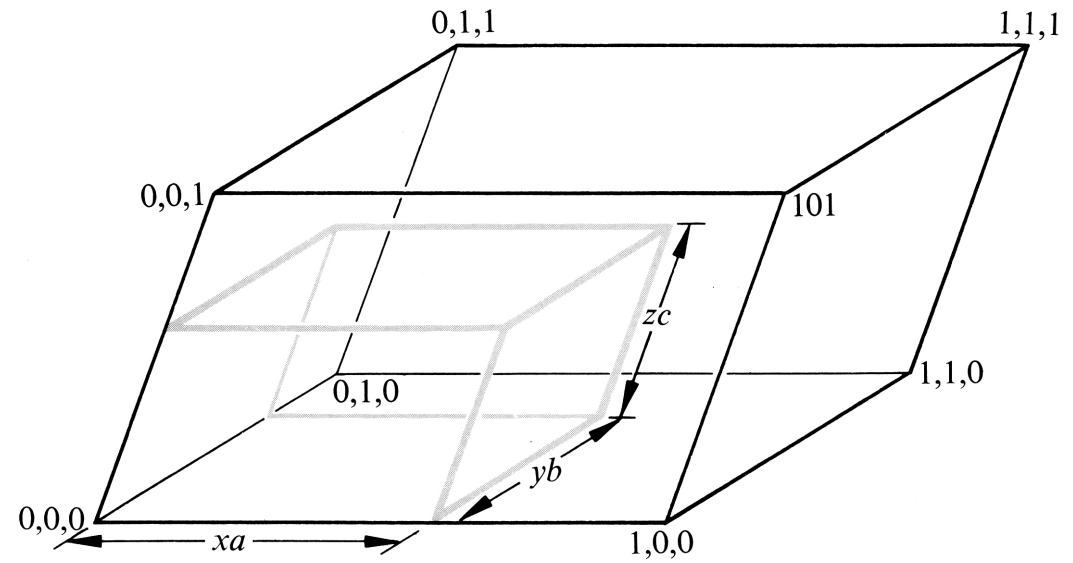
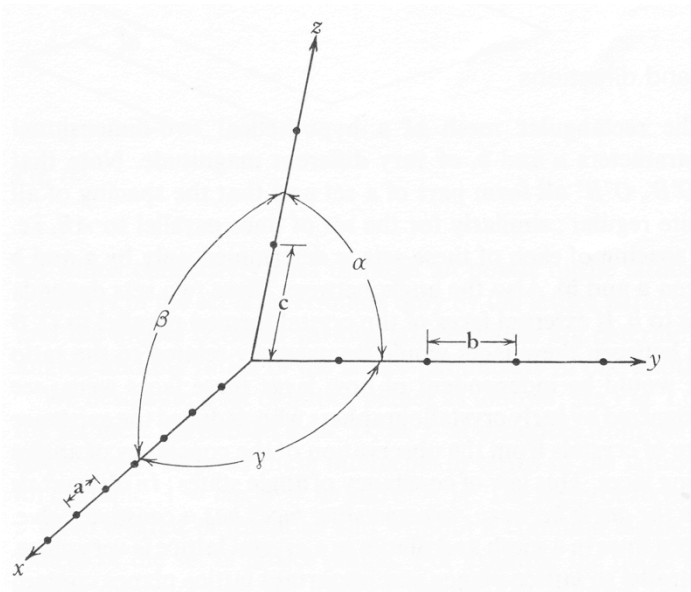
Crystal system	Point group	Space groups
Triclinic	$\bar{1}$	P1
	1	P1
Monoclinic	$\bar{2}$	P2, P2 ₁ , C2
	<i>m</i>	Pm, Pc, Cm, Cc
	2/m	P2/m, P2 ₁ /m, C2/m, P2/c, P2₁/c , C2/c
Orthorhombic	$\bar{2}22$	P222, P222₁ , P2₁2₁2 , P2₁2₁2₁ , C222₁ , C222, F222, I222, I2 ₁ 2 ₁ 2 ₁
	<i>mm2</i>	Pmm2, Pmc2 ₁ , Pcc2, Pma2 ₁ , Pca2 ₁ , Pnc2 ₁ , Pmn2 ₁ , Pba2, Pna2 ₁ , Pnn2, Cmm2, Cmc2 ₁ , Ccc2, Amm2, Abm2, Ama2, Aba2, Fmm2, Fdd2 , <i>Immi2</i> , Iba2, Ima2
	<i>mmm</i>	Pmmm, Pnnn , Pccm, Pban , Pmma, Pnna , Pnma, Pcca, Pbam, Pccn , Pbcm, Pnmm, Pmmm, Pbcn , Pbca , Pnma, Cmcm, Cmca, Cmmm, Cccm, Cmma, Ccca , Fmmm, Fddd , Immm, Ibam, Ibca , Imma
Tetragonal	$\bar{4}$	P4, P4₁ , P4 ₂ , P4₃ , I4, I4₁
	4	P4, I4
	4/m	P4/m, P4 ₂ /m, P4/n , P4₂/n , I4/m, I4₁/a
	$\bar{4}22$	P422, P4 ₂ 12, P4 ₁ 22, P4₁2₁2 , P4₂22 , P4₂2₁2 , P4₃22 , P4₃2₁2 , I422, I4₁22
	4mm	P4mm, P4bm, P4 ₂ cm, P4 ₂ nm, P4cc, P4nc, P4 ₂ mc, P4 ₂ bc, I4mm, I4cm, I4md, I4cd
	$\bar{4}m$	P42m, P4 ₂ c, P4 ₂ m, P4₂1c , P4m2, P4c2, P4b2, P4n2, I4m2, I4c2, I42m, I42d
4/mmm	P4/mmm, P4/mcc, P4/nbm , P4/nnc , P4/mbm, P4/mnc, P4/nmm , P4/ncc , P4 ₂ /mmc, P4 ₂ /mcm, P4₂/nbc , P4₂/nmm , P4 ₂ /mbc, P4 ₂ /mmm, P4₂/nmc , P4₂/ncm , I4/mmm, I4/mcm, I4₁/amd , I4₁/acd	
Trigonal-hexagonal	$\bar{3}$	P3, P3₁ , P3 ₂ , R3
	3	P3, R3
	$\bar{3}2$	P312, P321, P3₁12 , P3₂12 , P3₂21 , R32
	3m	P3m1, P31m, P3c1, P31c, R3m, R3c
	$\bar{3}m$	P31m, P31c, P3m1, P3c1, R3m, R3c
	$\bar{6}$	P6, P6₁ , P6₅ , P6 ₃ , P6₂ , P6₄
	6	P6
	6/m	P6/m, P6 ₃ /m
	$\bar{6}22$	P622, P6₁22 , P6₅22 , P6₂22 , P6₄22 , P6₃22
	6mm	P6mm, P6cc, P6 ₃ cm, P6 ₃ mc
$\bar{6}m$	P6m2, P6c2, P62m, P62c	
6/mmm	P6/mmm, P6/mcc, P6 ₃ /mcm, P6 ₃ /mmc	
Cubic	$\bar{2}3$	P23, F23, I23, P2₁3 , I2 ₁ 3
	$m\bar{3}$	Pm3, Pn3 , Fm3, Fd3 , <i>Im3</i> , Pa3 , Ia3
	$\bar{4}32$	P432, P4₃32 , F432, F4₃32 , I432, P4₃32 , P4₁32 , I4₁32
	43m	P43m, F43m, I43m, P43n, F43c, I43d
	$m\bar{3}m$	Pm3m, Pn3n , Pm3n, Pn3m , Fm3m, Fm3c, Fd3m , Fd3c , <i>Im3m</i> , Ia3d

Space groups (and enantiomorphous pairs) that are uniquely determinable from the symmetry of the diffraction pattern and from systematic absences (see Section 3.13.5) are shown in bold-type. Point groups without inversion centres or mirror planes are emphasized by boxes.

The direct space

- The positions of atoms in crystals is the most fundamental information we need.
- Atoms in crystals physically exist in real or direct space where the atoms positions are described relative to an origin, typically at a corner, in 3-D volume called the “unit cell”.
- The 3 axes of the unit cell x , y and z form a right-handed set with angles α (α), β (β) and γ (γ) between y - z , x - z and x - y respectively. The lattice parameters, a , b , c describe the dimensions of the unit cell along x , y and z .

Unit Cell Fractional Coordinates



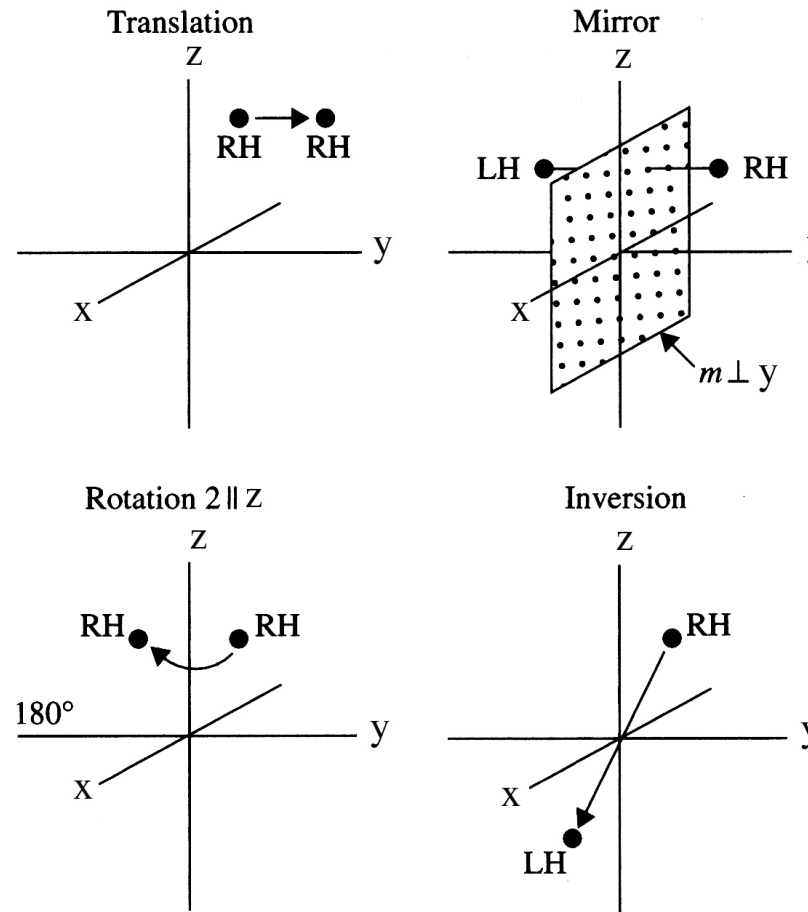
Location of a point with coordinates x,y,z . Numbers indicate coordinates of unit cell corners.

Example for alpha-quartz

- UNIT CELL DATA
- a: 4.9137 b: 4.9137 c: 5.4047 A
- alpha: 90.000 beta: 90.000 gamma: 120.000 degrees
-
- cell volume: 113.011 A**3
- calculated density: 2648.86 kg / m**3
-
- RECIPROCAL UNIT CELL DATA
-
- a*: 0.2350 b*: 0.2350 c*: 0.1850 1/A
- alpha*: 90.000 beta*: 90.000 gamma*: 60.000 degrees
-
- Space Group Symbol: P 32 2 1
-
- ASYMMETRIC UNIT
-
- -----
- label Site Occupancy x y z Num In Cell
- -----
- O O 1.000 0.4133 0.2672 0.1188 6
- T Si 1.000 0.4697 0.0000 0.0000 3
- -----
-
- Total of: 9 atoms in the unit cell

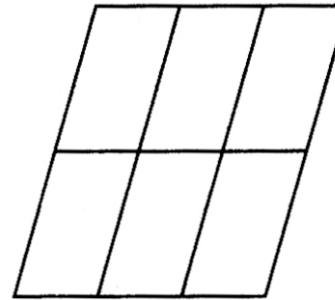
Four types of symmetry operation

Four types of symmetry elements.
Mirror and inversion transformation are accompanied by a handedness change; rotations and translations are not.

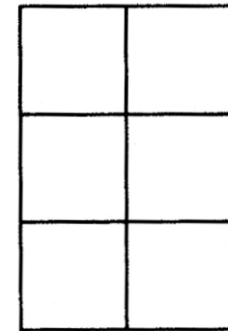


Space filling patterns

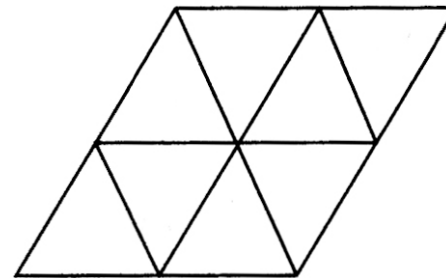
- 2-D space filling pattern for $n=2,3,4$ and 6-fold symmetry for $360^\circ/n$ rotations, used in combination with translation, mirror and inversion to generate the 32 3-D space filling point groups
- Note that 5-fold symmetry is found in quasicrystalline metal alloys, but they do not have the translation periodicity of single crystals, first observed in 1984.
- Do natural quasicrystalline minerals exist ?



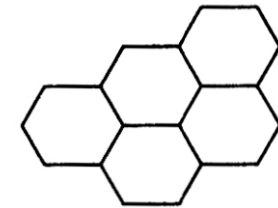
2-Fold (180°)



4-Fold (90°)



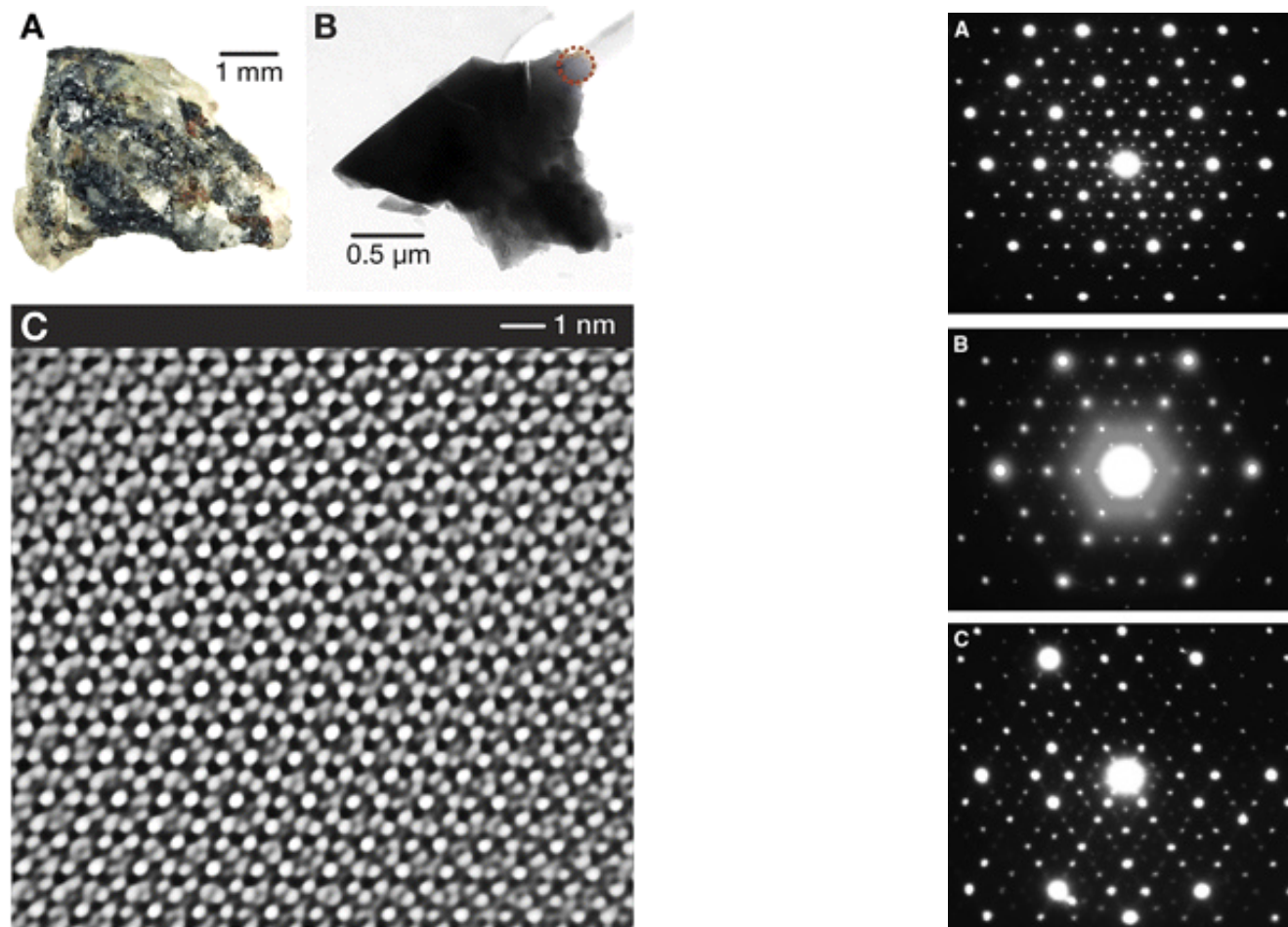
3-Fold (120°)



6-Fold (60°)

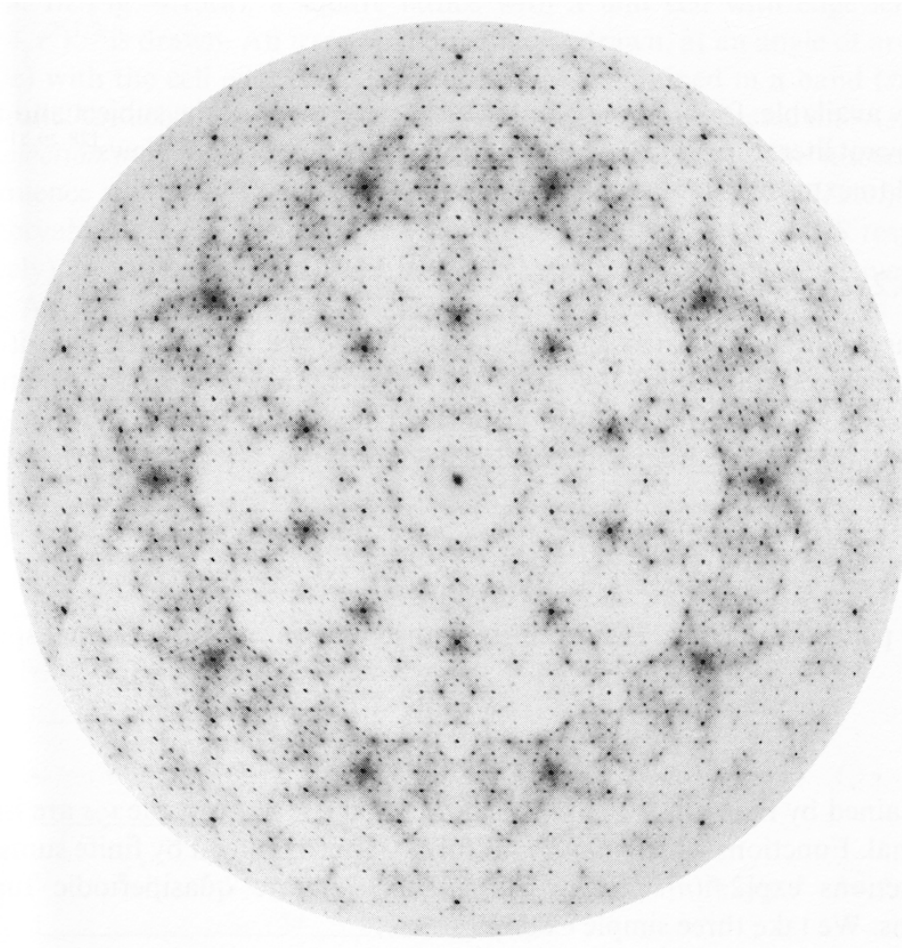
Planar figures with 2-, 3-, 4-, or 6-fold symmetry generate geometric patterns that fill space.

Natural quasicrystal : $\text{Al}_{63}\text{Cu}_{24}\text{Fe}_{13}$



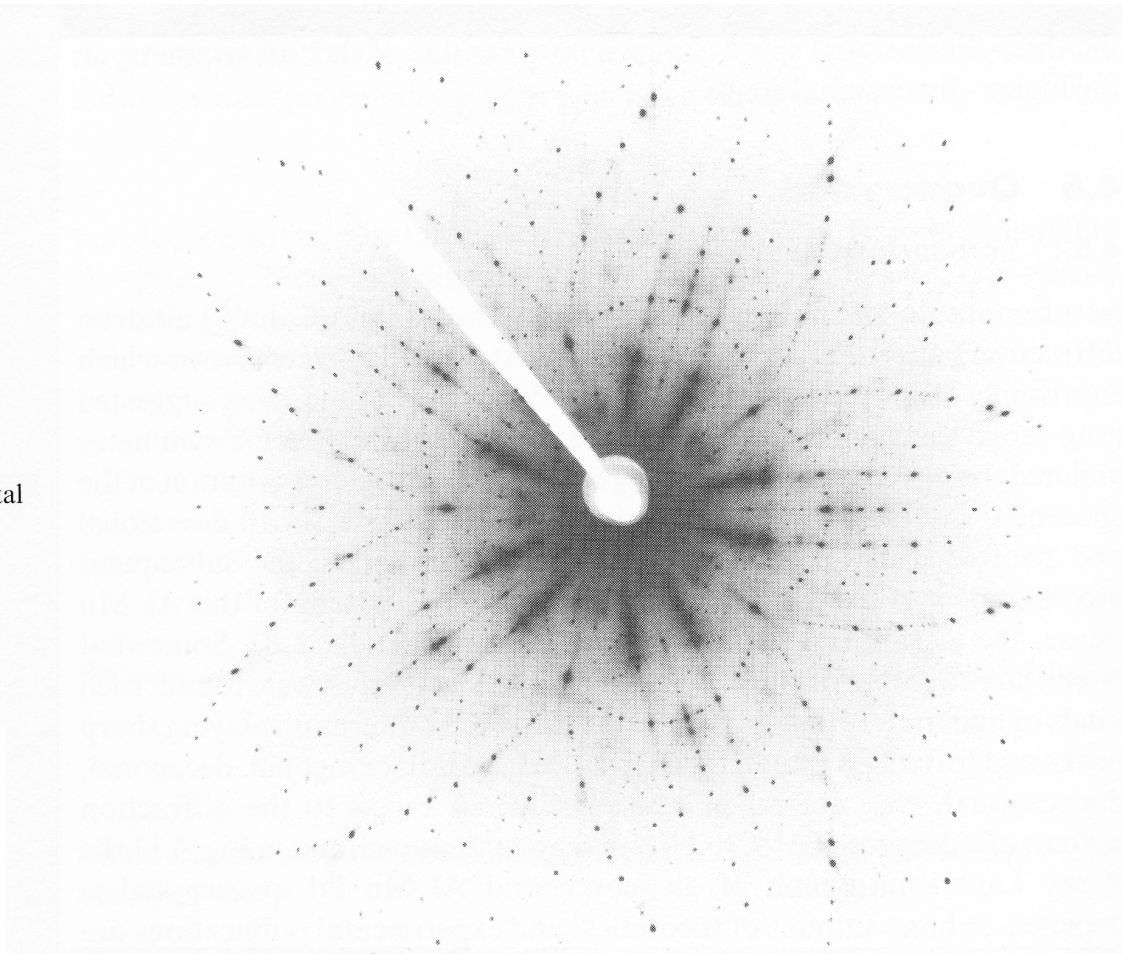
LEFT: Fig. 1 (A) The original khatyrkite-bearing sample used in the study. The lighter-colored material on the exterior contains a mixture of spinel, augite, and olivine. The dark material consists predominantly of khatyrkite (CuAl_2) and cupalite (CuAl) but also includes granules, like the one in (B), with composition $\text{Al}_{63}\text{Cu}_{24}\text{Fe}_{13}$. The diffraction patterns in Fig. 4 were obtained from the thin region of this granule indicated by the red dashed circle, an area $0.1 \mu\text{m}$ across. (C) The inverted Fourier transform of the HRTEM image taken from a subregion about 15 nm across displays a homogeneous, quasiperiodically ordered, fivefold symmetric, real space pattern characteristic of quasicrystals.

RIGHT: Diffraction patterns obtained from natural quasicrystal grain

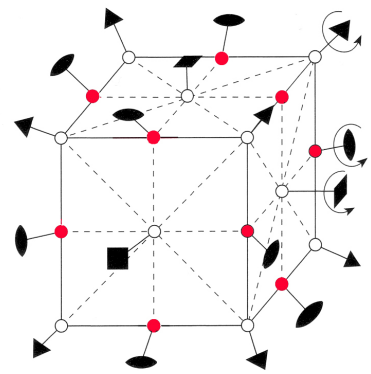
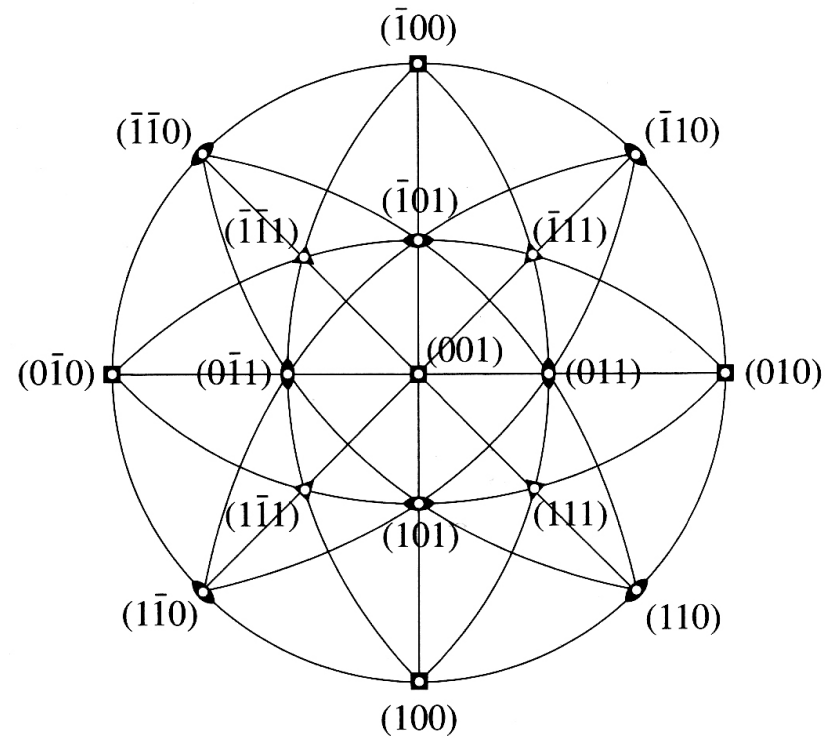
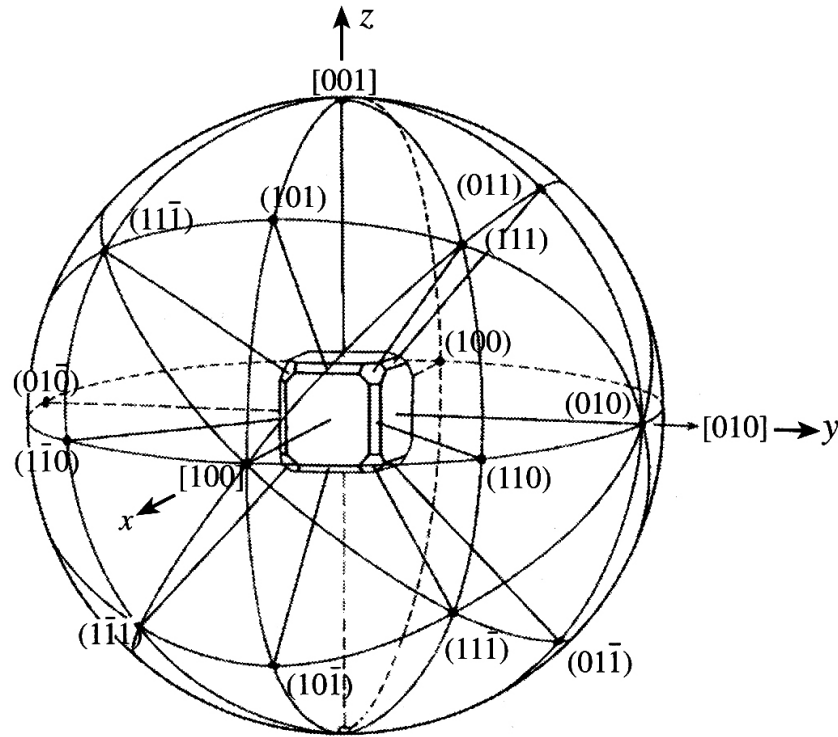


Diffraction pattern of a decagonal Al-Co-Ni quasicrystal. A computer reconstruction of the second layer from 720 images. Recorded with monochromatic X-rays (0.873 \AA) on a MARRESEARCH imaging plate detector system at the Swiss-Norwegian beamline (SNBL) of the ESRF, Grenoble, France. (By courtesy of W. Steurer and M. Estermann.)

X-ray Laue photograph of n icosahedral Al-Mn-Pd quasicrystal with fivefold symmetry (Mo X-ray tube, 50 kV, 35 mA, 60 mm crystal-to-detector distance, 16 h exposure time, crystal by courtesy of Marc deBoisseau). (By courtesy of W. Steurer.)



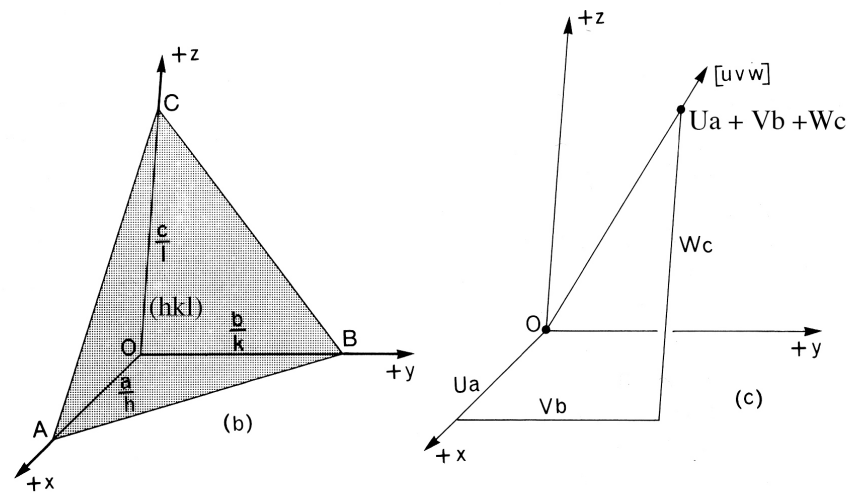
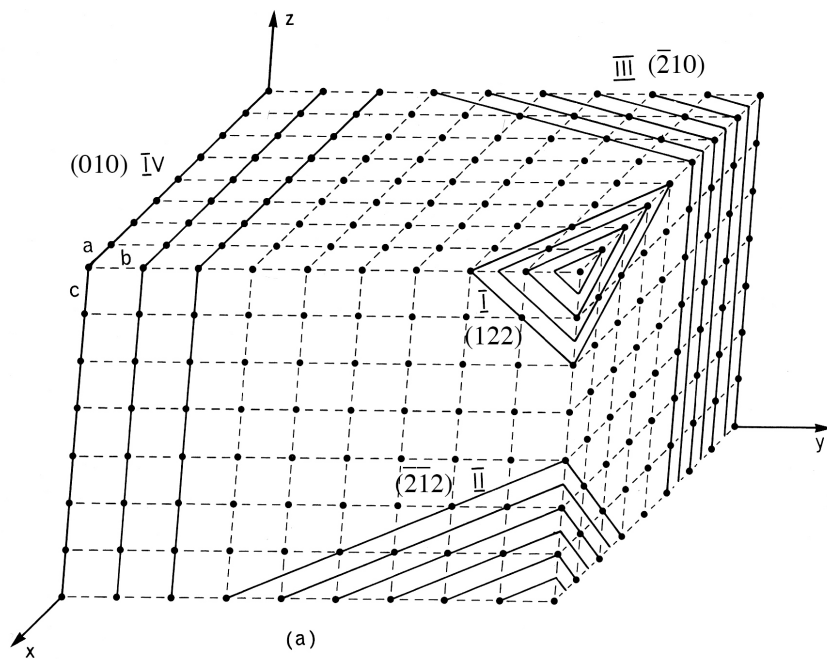
3D and Stereogram for Cubic symmetry



○ Cl⁻
● Na⁺

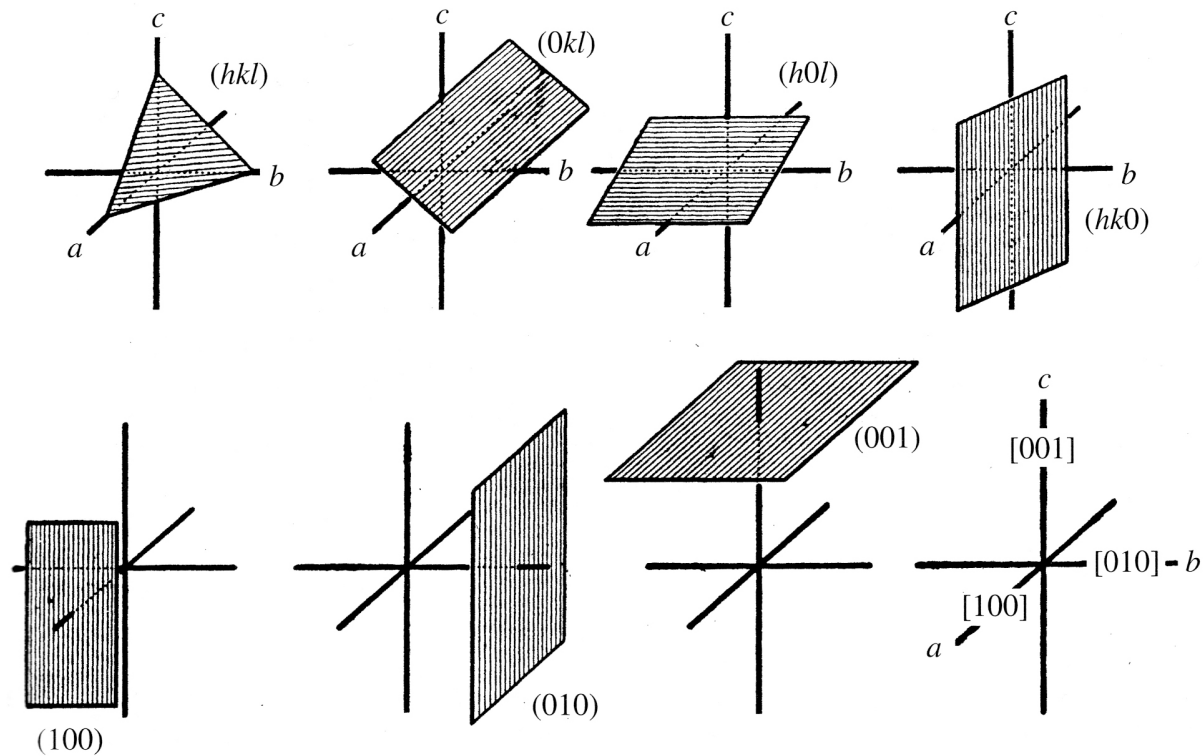
◐ = diad ; ▲ = triad ; ◆ = tetrad ; ● = hexad.

Lattice – planes and directions

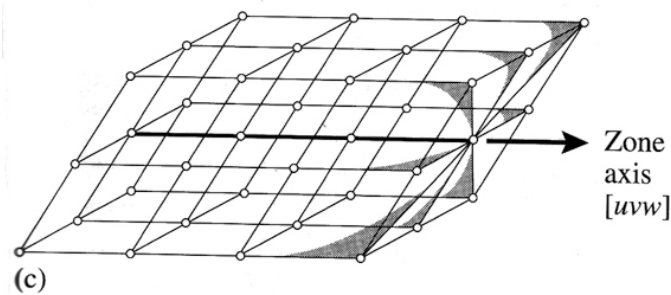
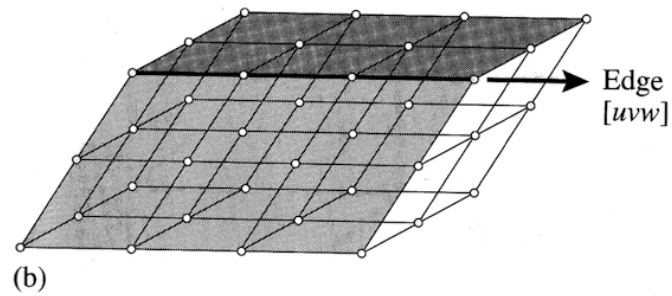
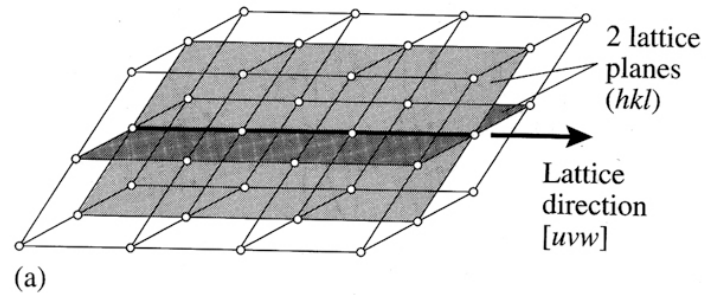


Lattice planes and zone axes. The array of lattice points exposed on the three visible faces of a parallelepiped whose edges are parallel to those of the unit-cell is displayed in (a) with solid circles to represent lattice points and thin broken lines parallel to axial directions. Four sets of lattice planes are indicated by thick solid lines representing the intersection of lattice planes with the visible faces of the parallelepiped; their Miller indices are I (122), II ($2\bar{1}2$), III ($2\bar{1}0$), IV (010). In (b) the definition of Miller indices is illustrated: the shaded plane (hkl) makes intercepts a/h , b/k , c/l on the x , y , z axes, a , b , c being the lattice repeat along each axis and h , k , l being integers. In (c) the definition of the zone axis symbol is illustrated: $[UVW]$ is the direction parallel to the line through the origin and the point Ua , Vb , Wc .

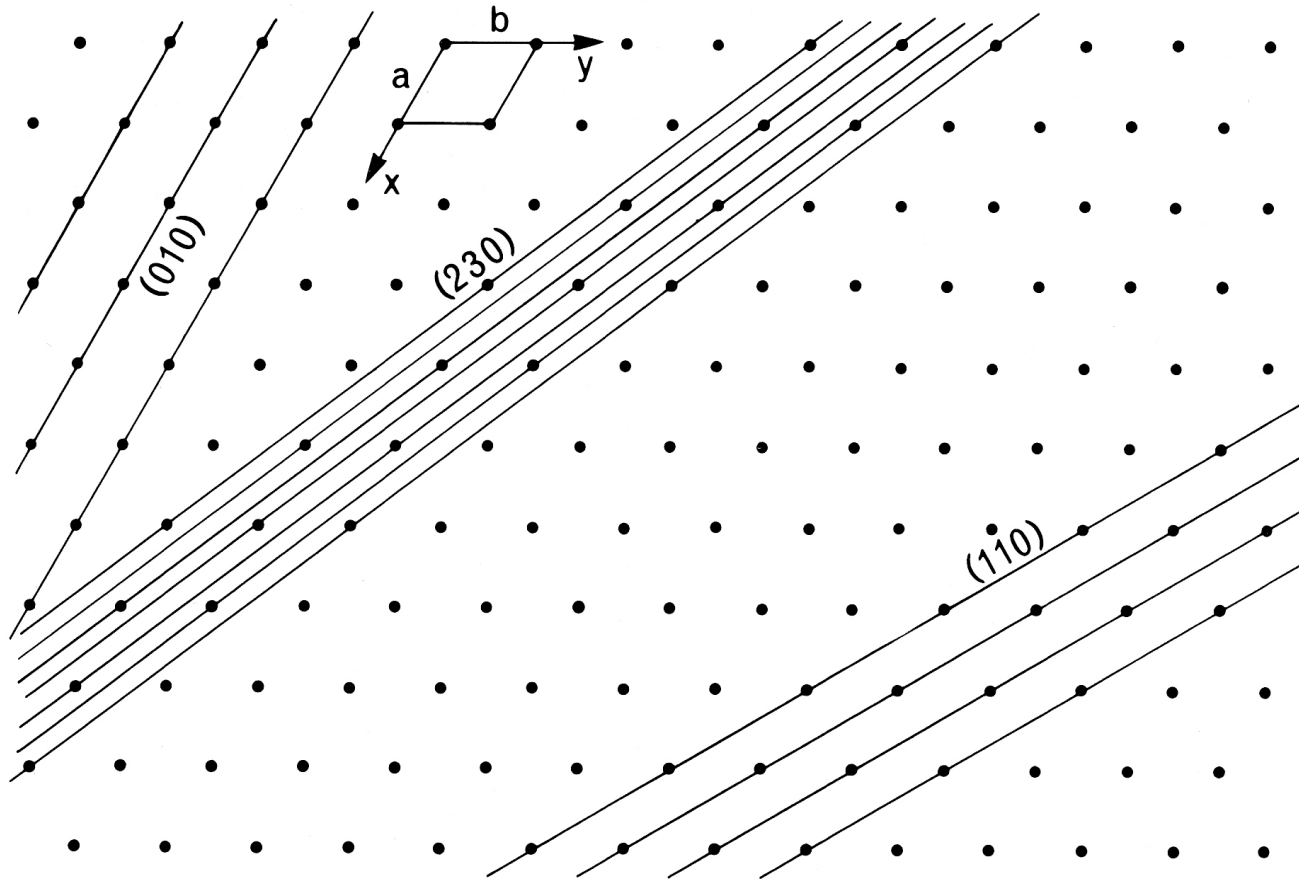
Typical planes and their Miller indices



Typical lattice directions



Lattice planes - Graphite [001] axis



Projection of the lattice of graphite down the z-axis on to the xy plane to illustrate the decrease in the density of lattice points per unit area of lattice planes ($hk0$) as their indices h and k increase. The density of lattice points per unit length in projection decreases from (010) to (110) to (230).

32 Point Groups

List of the 32 point groups

Crystal systems	Point groups		Laue classes	Lattice point groups
	Non-centro-symmetric	Centrosymmetric		
Triclinic	1	$\bar{1}$	$\bar{1}$	$\bar{1}$
Monoclinic	2 m	$2/m$	$2/m$	$2/m$
Orthorhombic	222 $mm2$	mmm	mmm	mmm
Tetragonal	[4 4 422 $4mm, \bar{4}2m$	$4/m$ $4/mmm$	$4/m$ $4/mmm$] $4/mmm$
Trigonal	[3 32 $3m$	$\bar{3}$ $\bar{3}m$	$\bar{3}$ $\bar{3}m$] $\bar{3}m$
Hexagonal	[6 $\bar{6}$ 622 $6mm, \bar{6}2m$	$6/m$ $6/mmm$	$6/m$ $6/mmm$] $6/mmm$
Cubic	[23 432 $\bar{4}3m$	$m\bar{3}$ $m\bar{3}m$	$m\bar{3}$ $m\bar{3}m$] $m\bar{3}m$

7 Crystal Symmetry systems

- *Triclinic*. No symmetry other than translational symmetry
- *Monoclinic*. One twofold rotation axis or one mirror plane
- *Orthorhombic*. Three twofold rotation axes or one twofold rotation axis and two mirror planes
- *Tetragonal*. One fourfold rotation axis
- *Rhombohedral (also called trigonal)*. One threefold rotation axis
- *Hexagonal*. One sixfold rotation axis
- *Cubic (also called isometric)*. Four threefold rotation axes

Frequency of different point groups

Table Population statistics for the 32 crystallographic point groups gathered from more than 280,000 chemical compounds. Inorganic (I) and organic (O) have somewhat different percentages (data collected by G. Johnson)

	I	O		I	O
1	0.67%	1.24%	422	0.40%	0.48%
1	13.87	19.18	4mm	0.30	0.09
2	2.21	6.70	$\bar{4}2m$	0.82	0.34
<i>m</i>	1.30	1.46	4/mmm	4.53	0.69
2/m	34.63	44.81	6	0.41	0.22
222	3.56	10.13	$\bar{6}$	0.07	0.01
<i>mm2</i>	3.32	3.31	6/m	0.82	0.17
<i>mmm</i>	12.07	7.84	622	0.24	0.05
3	0.36	0.32	6mm	0.45	0.03
$\bar{3}$	1.21	0.58	$\bar{6}m2$	0.41	0.02
32	0.54	0.22	6/mmm	2.82	0.05
3 <i>m</i>	0.74	0.22	23	0.44	0.09
$\bar{3}m$	3.18	0.25	<i>m3</i>	0.84	0.15
4	0.19	0.25	432	0.13	0.01
$\bar{4}$	0.25	0.18	$\bar{4}3m$	1.42	0.11
4/m	1.17	0.67	<i>m3m</i>	6.66	0.12

metals

Examples of 32 point groups

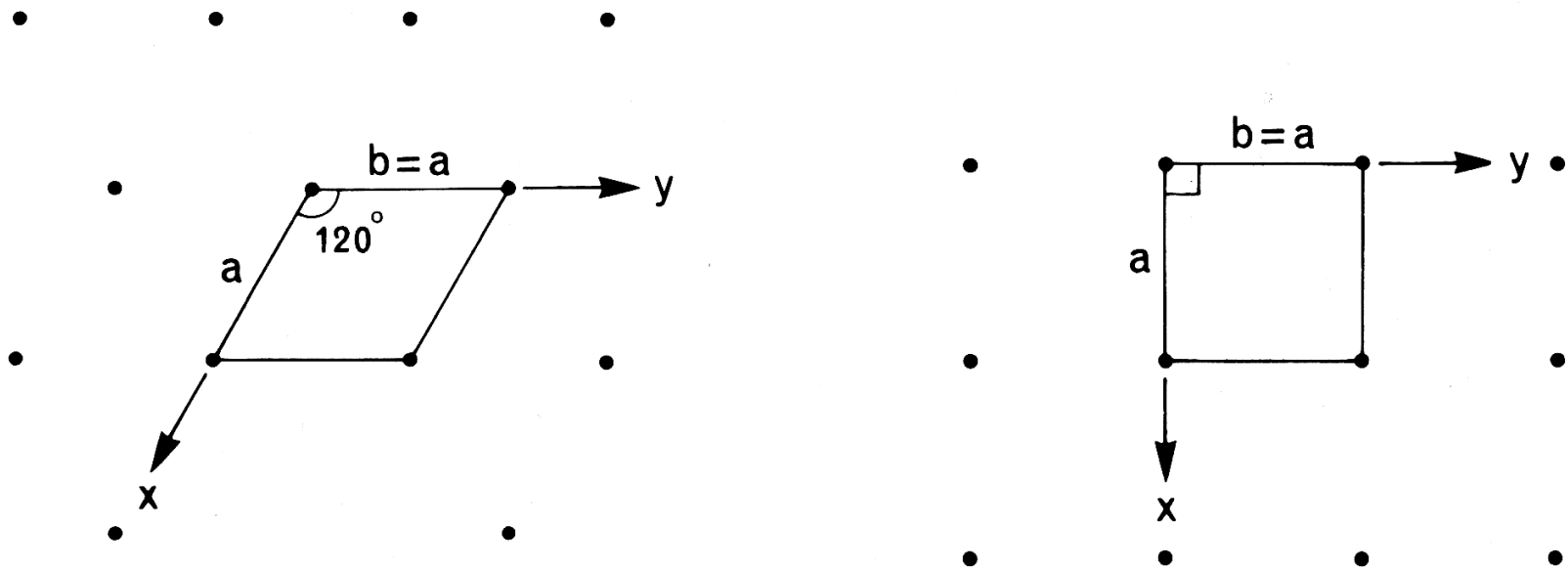
Table Examples of the 32 crystal classes

$1 = C_1$	Kaolinite	$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$
$\bar{1} = C_i$	Copper sulfate	$\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
$2 = C_2$	Sucrose	$\text{C}_{12}\text{H}_{22}\text{O}_{11}$
$m = C_s$	Potassium nitrite	KNO_2
$2/m = C_{2h}$	Orthoclase	KAlSi_3O_8
$222 = D_2$	Iodic acid	HIO_3
$mm2 = C_{2v}$	Sodium nitrite	NaNO_2
$mmm = D_{2h}$	Forsterite	Mg_2SiO_4
$3 = C_3$	Nickel tellurate	Ni_3TeO_6
$\bar{3} = C_{3i}$	Ilmenite	FeTiO_3
$32 = D_3$	Low-quartz	SiO_2
$3m = C_{3v}$	Lithium niobate	LiNbO_3
$\bar{3}m = D_{3d}$	Corundum	Al_2O_3
$4 = C_4$	Iodosuccinimide	$\text{C}_4\text{H}_4\text{INO}_2$
$\bar{4} = S_4$	Boron phosphate	BPO_4
$4/m = C_{4h}$	Scheelite	CaWO_4
$422 = D_4$	Nickel sulfate	$\text{NiSO}_4 \cdot 6\text{H}_2\text{O}$
$4mm = C_{4v}$	Barium titanate	BaTiO_3
$\bar{4}2m = D_{2d}$	Potassium dihydrogen phosphate	KH_2PO_4
$4/mmm = D_{4h}$	Rutile	TiO_2
$6 = C_6$	Nepheline	$\text{NaAlSi}_3\text{O}_8$
$\bar{6} = C_{3h}$	Lead germanate	$\text{Pb}_5\text{Ge}_3\text{O}_{11}$
$6/m = C_{6h}$	Apatite	$\text{Ca}_5(\text{PO}_4)_3\text{F}$
$622 = D_6$	High-quartz	SiO_2
$6mm = C_{6v}$	Zincite	ZnO
$\bar{6}m2 = D_{3h}$	Benitoite	$\text{BaTiSi}_3\text{O}_9$
$6/mmm = D_{6h}$	Beryl	$\text{Be}_3\text{Al}_2\text{Si}_6\text{O}_{18}$
$23 = T$	Sodium chlorate	NaClO_3
$m3 = T_h$	Pyrite	FeS_2
$432 = O$	Manganese	$\beta\text{-Mn}$
$\bar{4}3m = T_d$	Zincblende	ZnS
$m3m = O_h$	Rocksalt	NaCl

Symmetry

- The defining property of a crystal is its inherent symmetry, which means that certain operations result in an atomic configuration identical to the original configuration. For example, rotating the crystal by 90° or 180° about a certain axis may leave the crystal unchanged. The crystal is then said to have, respectively, a fourfold or twofold rotational symmetry about this axis.
- In addition to rotational symmetries like this, a crystal may have symmetries in the form of mirror planes and translational symmetries, and also the so-called compound symmetries that are a combination of translation and rotation/mirror symmetries. A full classification of a crystal is achieved when all of these inherent symmetries of the crystal are identified.
- A crystal lattice is conveniently described by its unit cell, a tiny box containing one or more atoms, which is characterized by its lattice parameters a , b , and c as well as the angles α , β , and γ between them. There may be additional lattice points at the center of certain faces or at the center of volume within the unit cell. The positions of the atoms inside the unit cell are described by the set of atomic positions (x_i, y_i, z_i) measured from the origin, a lattice point at the corner of the unit cell.
- There are only seven possible crystal systems that atoms can pack together to produce an infinite 3-D space lattice in such a way that each lattice point has an identical environment to that around every other lattice point. The crystal systems are a grouping of crystal structures according to the axial system used to describe their lattice.

Example of invariant patterns – 120° and 90° rotations



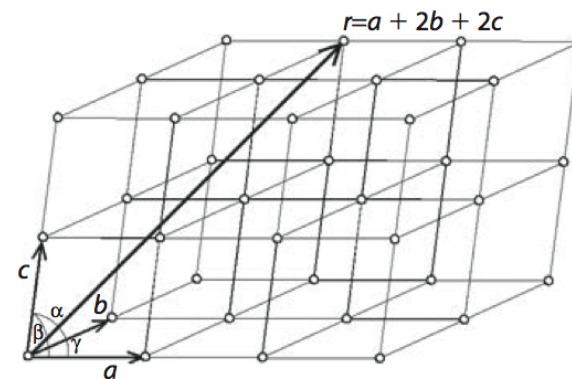
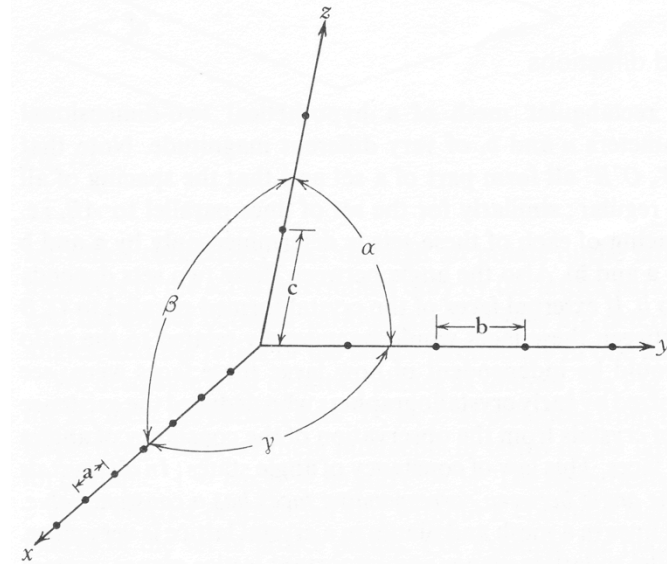
Two-dimensional lattices with (a) a triad or a hexad, (b) a tetrad perpendicular to the plane of the lattice.

Lattice

- A lattice is an infinite set of points generated by a set of discrete translation operations. A crystal is made up of one or more atoms that are repeated at each lattice point.
- For minerals, the lattice points contain identical groups of atoms, called a motif (or basis) of atoms. That is to say, the crystal structure consists of the same atoms, or motifs, positioned around each and every lattice point. This group of atoms, therefore, repeats indefinitely in three dimensions according to the arrangement of the crystal lattices.
- In total, there are 14 lattices that fill the 3-D space, which are the well-known 14 Bravais lattices. The characteristic rotation and mirror symmetries of the atoms or motifs are described by the crystallographic point groups, of which there are 32, and space groups, of which there are 230.

Direct space – unit cell

- The unit cell may be primitive containing one lattice point referred to the primitive basis, \mathbf{a} , \mathbf{b} , \mathbf{c} .
- A non-primitive unit cell contains multiple lattice points referred to the crystallographic basis, \mathbf{a}_c , \mathbf{b}_c , \mathbf{c}_c by adding lattice nodes at the center of the unit cell using 'centring vectors'. Examples include A, B, and C face centered, body centered, rhombohedrally and hexagonally centred.

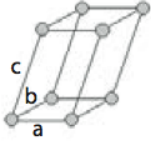
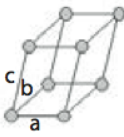
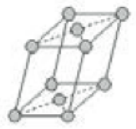
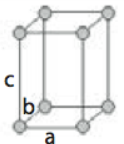
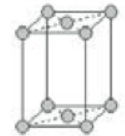
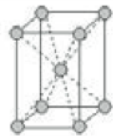
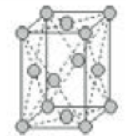
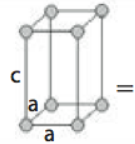
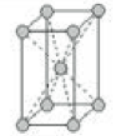
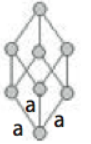
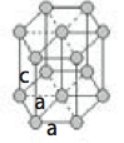
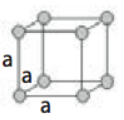




14 Bravais lattices (or space lattices)

'centring vectors'

- Primitive (P). Lattice points on the cell corners only, that is, at the coordinates $(x,y,z) = (0,0,0)$
- Body centered (I). One additional lattice point at the center of the cell so that for each atom at $(0,0,0)$ there is another one at $(1/2,1/2,1/2)$
- Face centered (F). One additional lattice point at the center of each of the faces of the cell, that is, there are also atoms at $(1/2,1/2,0)$, $(1/2,0,1/2)$, and $(0,1/2,1/2)$
- Base centered (C). One additional lattice point at the center of the base of the cell (the so-called C-plane containing a and b), that is, at $(1/2,1/2,0)$

14 Bravais lattices

Name	Conditions	Primitive	Base centered	Body centered	Face centered
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$				
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$				
Orthomombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$				
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$				
Rhombohedral (trigonal)	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$				
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$				
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$				

Crystallographic calculations

Structure factor - amplitude and phase of diffracted wave

- The **structure factor** is a mathematical function describing the amplitude and phase of a wave diffracted from crystal lattice planes characterised by Miller indices (hkl)

- The structure factor may be expressed as

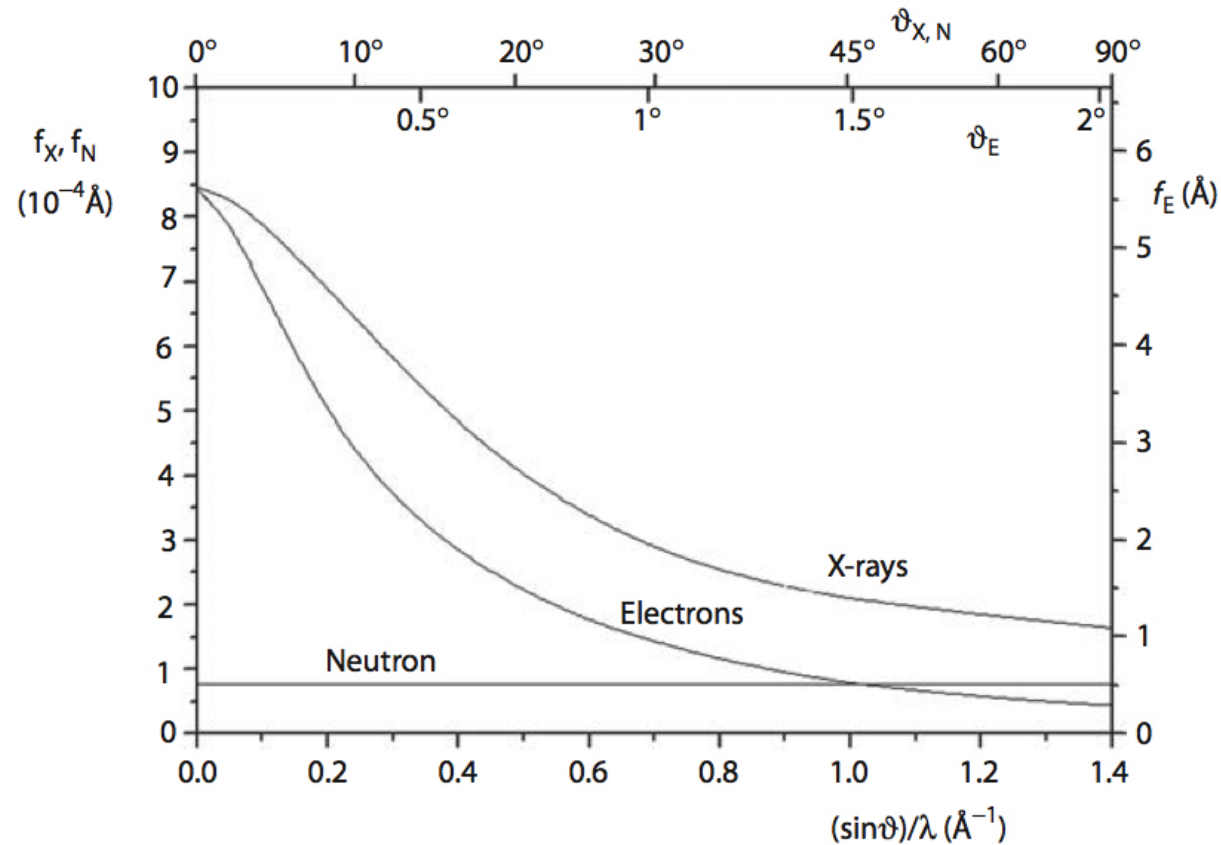
$$\begin{aligned}\mathbf{F}_{hkl} &= F_{hkl} \exp(i\alpha_{hkl}) = \sum_j f_j \exp[2\pi i(hx_j + ky_j + lz_j)] \\ &= \sum_j f_j \cos[2\pi(hx_j + ky_j + lz_j)] + i \sum_j f_j \sin[2\pi(hx_j + ky_j + lz_j)] \\ &= A_{hkl} + iB_{hkl}\end{aligned}$$

where the sum is over all atoms in the unit cell, x_j, y_j, z_j are the positional coordinates of the j th atom, f_j is the scattering factor of the j th atom (is measure of the scattering power of an isolated atom and is specific for each atom Mg, Ca, Fe etc, their charge state Fe^{2+} , Fe^{3+} , and radiation, x-rays, neutrons or electrons) 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 $|F_{hkl}| = ((A_{hkl})^2 + (B_{hkl})^2)^{1/2}$, where as the phase is given by $\tan(\text{phase angle}) = B_{hkl}/A_{hkl}$

Most recent reference for electrons is 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 doi: 10.1107/97809553602060000593

Atomic scattering amplitudes for Cu



Angular variation of the atomic scattering amplitude f of copper for x-rays, electrons, and neutrons (note different scales for electrons). The reflection angles of the upper axis were calculated with $\lambda = 0.07107$ nm for x-rays and neutrons, and with $\lambda = 0.00251$ nm for electrons (see Table 3.1). (Data for x-rays and electrons taken from Doyle, P.A. and Turner, P.S., *Acta Crystallogr.*, A24, 390, 1968; data for neutrons taken from Bacon, G.E., *Neutron Diffraction*, Clarendon Press, Oxford, 1975.)

Example alpha-Quartz

• REFLEXIONS

ref no.	h	k	l	d [Å]	d* [1/Å]	F(Real)	F(Imaginary)	F	Phase [deg]	I/Imax
[1]	-1	1	-1	3.3434	0.29909	-2.0643e+05	-3.5754e+05	4.1285e+05	240.00	100.000%
[2]	1	-1	1	3.3434	0.29909	-2.0643e+05	3.5754e+05	4.1285e+05	120.00	100.000%
[3]	0	1	1	3.3434	0.29909	4.1285e+05	5.7203e-02	4.1285e+05	0.00	100.000%
[4]	0	-1	-1	3.3434	0.29909	4.1285e+05	-5.7203e-02	4.1285e+05	0.00	100.000%
[5]	1	0	-1	3.3434	0.29909	-2.0643e+05	3.5754e+05	4.1285e+05	120.00	100.000%
[6]	-1	0	1	3.3434	0.29909	-2.0643e+05	-3.5754e+05	4.1285e+05	240.00	100.000%
[7]	1	-1	-1	3.3434	0.29909	-1.3703e+05	-2.3735e+05	2.7407e+05	240.00	44.067%
[8]	-1	1	1	3.3434	0.29909	-1.3703e+05	2.3735e+05	2.7407e+05	120.00	44.067%
[9]	0	-1	1	3.3434	0.29909	2.7407e+05	1.9396e-02	2.7407e+05	0.00	44.067%
[10]	0	1	-1	3.3434	0.29909	2.7407e+05	-1.9396e-02	2.7407e+05	0.00	44.067%
[11]	-1	0	-1	3.3434	0.29909	-1.3703e+05	2.3735e+05	2.7407e+05	120.00	44.067%
[12]	1	0	1	3.3434	0.29909	-1.3703e+05	-2.3735e+05	2.7407e+05	240.00	44.067%
[13]	0	2	-3	1.3749	0.72732	2.2390e+05	-6.1543e-03	2.2390e+05	0.00	29.401%
[14]	0	-2	3	1.3749	0.72732	2.2390e+05	6.1543e-03	2.2390e+05	0.00	29.401%
[15]	2	-2	-3	1.3749	0.72732	2.2390e+05	2.1561e-02	2.2390e+05	0.00	29.401%
[16]	-2	2	3	1.3749	0.72732	2.2390e+05	-2.1561e-02	2.2390e+05	0.00	29.401%
[17]	2	0	3	1.3749	0.72732	2.2390e+05	2.1592e-02	2.2390e+05	0.00	29.401%
[18]	-2	0	-3	1.3749	0.72732	2.2390e+05	-2.1592e-02	2.2390e+05	0.00	29.401%

The reciprocal lattice concept : 1

A concept is a cognitive unit of meaning - an abstract idea or a mental symbol

The notion of reciprocal vectors was introduced into vector analysis by J. W. Gibbs (1881). The concept of reciprocal space or reciprocal lattice was adapted by P. P. Ewald to interpret the diffraction patterns of an orthorhombic crystal (1913). The concept is very useful for metric calculations and diffraction geometry. Let \mathbf{a} , \mathbf{b} , \mathbf{c} be the elementary translation vectors (i.e. associated with alpha, beta, gamma) of real space or direct lattice. The reciprocal lattice is defined by translation vectors \mathbf{a}^* , \mathbf{b}^* and \mathbf{c}^* , which satisfy the following conditions related to the direct space:

$$\mathbf{a}^* \cdot \mathbf{b} = \mathbf{a}^* \cdot \mathbf{c} = 0 \quad (\mathbf{a}^* \text{ is normal to } \mathbf{b} \text{ and } \mathbf{c})$$

$$\mathbf{b}^* \cdot \mathbf{a} = \mathbf{b}^* \cdot \mathbf{c} = 0 \quad (\mathbf{b}^* \text{ is normal to } \mathbf{a} \text{ and } \mathbf{c})$$

$$\mathbf{c}^* \cdot \mathbf{a} = \mathbf{c}^* \cdot \mathbf{b} = 0 \quad (\mathbf{c}^* \text{ is normal to } \mathbf{a} \text{ and } \mathbf{b})$$

and

$$\mathbf{a}^* \cdot \mathbf{a} = 1 \quad (\mathbf{a} = 1/\mathbf{a}^* \text{ these relations fix the direction and magnitude of } \mathbf{a}^* \text{ etc})$$

$$\mathbf{b}^* \cdot \mathbf{b} = 1 \quad (\mathbf{b} = 1/\mathbf{b}^*)$$

$$\mathbf{c}^* \cdot \mathbf{c} = 1 \quad (\mathbf{c} = 1/\mathbf{c}^*)$$

From these relations it follows that reciprocal vectors are

$$\mathbf{a}^* = (\mathbf{b} \times \mathbf{c}) / \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) \quad \mathbf{b}^* = (\mathbf{c} \times \mathbf{a}) / \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) \quad \mathbf{c}^* = (\mathbf{a} \times \mathbf{b}) / \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})$$

$$\text{As volume of the unit cell, } V = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})$$

$$\mathbf{a}^* = (\mathbf{b} \times \mathbf{c}) / V \quad \mathbf{b}^* = (\mathbf{c} \times \mathbf{a}) / V \quad \mathbf{c}^* = (\mathbf{a} \times \mathbf{b}) / V$$

With magnitudes

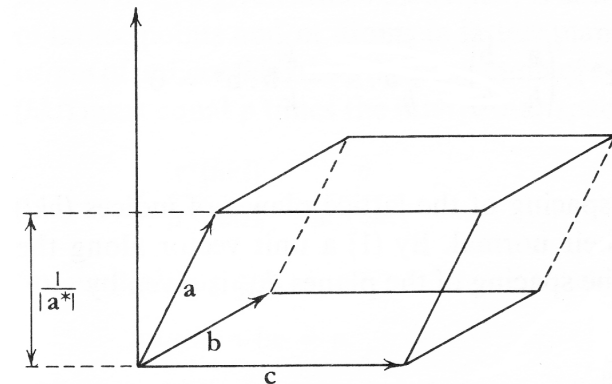
$$|\mathbf{a}^*| = bc \sin \alpha / V \quad |\mathbf{b}^*| = ca \sin \beta / V \quad |\mathbf{c}^*| = ab \sin \gamma / V$$

where $|\mathbf{a}^*|$ is equal **reciprocal** of the spacing of (100) planes, similarly for $|\mathbf{b}^*|$ and $|\mathbf{c}^*|$ for (010) and (001).

The roles of direct and reciprocal space may be interchanged: that is the “reciprocal” of the reciprocal lattice is the direct lattice ! Therefore

$$\mathbf{a} = (\mathbf{b}^* \times \mathbf{c}^*) / V \quad \mathbf{b} = (\mathbf{c}^* \times \mathbf{a}^*) / V \quad \mathbf{c} = (\mathbf{a}^* \times \mathbf{b}^*) / V$$

It may be easily verified that that reciprocal of direct triclinic lattice also has triclinic symmetry, but not is true for all lattice symmetry classes.



The reciprocal lattice concept : 2

Relations for specific symmetries

In **monoclinic lattices** $\mathbf{b}^* \parallel \mathbf{b}$ while \mathbf{a}^* and \mathbf{c}^* are in the plane (\mathbf{a}, \mathbf{c}) , then:

$$|\mathbf{a}^*| = 1/(a \sin \beta) \quad |\mathbf{b}^*| = 1/b \quad |\mathbf{c}^*| = 1/(c \sin \beta)$$

$$\alpha^* = \gamma^* = \pi/2 \quad \beta^* = \pi - \beta$$

In **orthorhombic, tetragonal and cubic lattices** $\mathbf{a}^* \parallel \mathbf{a}$, $\mathbf{b}^* \parallel \mathbf{b}$ and $\mathbf{c}^* \parallel \mathbf{c}$, then:

$$|\mathbf{a}^*| = 1/a \quad |\mathbf{b}^*| = 1/b \quad |\mathbf{c}^*| = 1/c$$

$$\alpha^* = \beta^* = \gamma^* = \pi/2$$

In **trigonal (hexagonal axes - recommended) and hexagonal lattices** $\mathbf{c}^* \parallel \mathbf{c}$ while \mathbf{a}^* and \mathbf{b}^* are in the plane (\mathbf{a}, \mathbf{b}) , then:

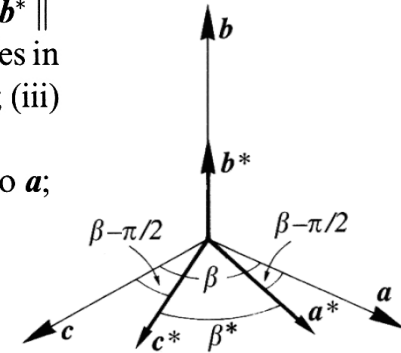
$$|\mathbf{a}^*| = |\mathbf{b}^*| = 2/(a\sqrt{3}) \quad |\mathbf{c}^*| = 1/c \quad \alpha^* = \beta^* = \pi/2$$

$$\gamma^* = \pi/3$$

(Note this will differ for trigonal lattices on rhombohedral axes)

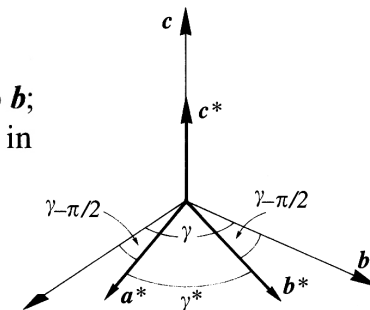
Direct and reciprocal lattice parameters for a monoclinic unit cell. We notice: (i) \mathbf{b}^* is normal to the plane (\mathbf{a}, \mathbf{c}) by definition, and therefore $\mathbf{b}^* \parallel \mathbf{b}$; (ii) \mathbf{a}^* is normal to \mathbf{b} , therefore lies in the plane (\mathbf{a}, \mathbf{c}) , and is normal to \mathbf{c} ; (iii) \mathbf{c}^* is normal to \mathbf{b} , therefore lies in the plane (\mathbf{a}, \mathbf{c}) , and is normal to \mathbf{a} ;

(iv) $\beta^* = \beta - (\beta - \pi/2) - (\beta - \pi/2)$
 $= \pi - \beta$



Direct and reciprocal lattice parameters for a trigonal (hexagonal) unit cell. We notice: (i) \mathbf{c}^* is normal to the plane (\mathbf{a}, \mathbf{b}) by definition, and therefore $\mathbf{c}^* \parallel \mathbf{c}$; (ii) \mathbf{a}^* is normal to \mathbf{c} , therefore lies in the plane (\mathbf{a}, \mathbf{b}) , and is normal to \mathbf{b} ; (iii) \mathbf{b}^* is normal to \mathbf{c} , therefore lies in the plane (\mathbf{a}, \mathbf{b}) , and is normal to \mathbf{a} ;

(iv) $\gamma^* = \gamma - (\gamma - \pi/2) - (\gamma - \pi/2)$
 $= \pi - \gamma = 60^\circ$.



The reciprocal lattice concept : 3

Some useful relationships

1. A lattice vector of the reciprocal lattice \mathbf{r}^*

$$\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

is normal to the the planes with Miller indices (hkl) in the **real or direct lattice**.

If the h,k,l have small integer values the plane is said to be “low index” plane (e.g. 100).

2. The magnitude of \mathbf{r}^* (i.e. $|\mathbf{r}^*| = 1/d_{hkl}$), is equal to the reciprocal of the spacing of the planes (d_{hkl}) of the **real lattice** with indices (hkl). The d_{hkl} is called the “d-spacing” in angstroms or nanometres.

Proof:

1. The vectors (A-O), (B-O) and (C-O) define the intercepts of the plane (hkl) at A with \mathbf{a}/h , B with \mathbf{b}/k and C with \mathbf{c}/l . The vectors along the triangular edges of plane (hkl) are therefore;

$$(\mathbf{B}-\mathbf{A}) = \mathbf{b}/k - \mathbf{a}/h \quad (\mathbf{C}-\mathbf{A}) = \mathbf{c}/l - \mathbf{a}/h \quad (\mathbf{C}-\mathbf{B}) = \mathbf{c}/l - \mathbf{b}/k$$

Hence

$$\mathbf{r}^* \cdot (\mathbf{B}-\mathbf{A}) = (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) \cdot (\mathbf{b}/k - \mathbf{a}/h) = h/h\mathbf{a}^* \cdot \mathbf{a}^* - k/k\mathbf{b}^* \cdot \mathbf{b}^* = 1 - 1 = 0$$

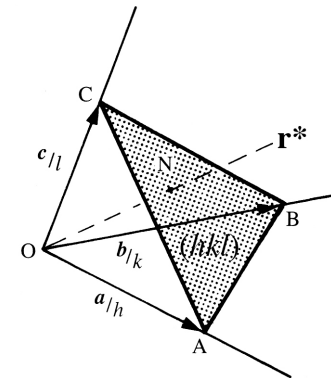
as $\mathbf{a} \cdot \mathbf{a}^* = \mathbf{b} \cdot \mathbf{b}^* = 1$ and $h/h = k/k = 1$

and therefore $\mathbf{r}^* \cdot (\mathbf{B}-\mathbf{A}) = \mathbf{r}^* \cdot (\mathbf{C}-\mathbf{A}) = \mathbf{r}^* \cdot (\mathbf{C}-\mathbf{B}) = 0$

Vectors (B-A), (C-A) and (C-B) are in the plane (hkl) and perpendicular to \mathbf{r}^*

2. Remembering that a dot product $\mathbf{AO} \cdot \mathbf{r}^*$ is equal to the projection of AO on the direction of \mathbf{r}^* multiplied by the magnitude of \mathbf{r}^* . If $\mathbf{n} = \mathbf{r}^*/|\mathbf{r}^*|$ is a unit vector parallel to ON and \mathbf{r}^* , then $\mathbf{OA} \cdot \mathbf{n}$ is the projection of AO in the direction of n,

$$d_{hkl} = \mathbf{OA} \cdot \mathbf{n} = (\mathbf{a}/h) \cdot (\mathbf{r}^*/|\mathbf{r}^*|) = h \mathbf{a} \cdot \mathbf{a}^* / h |\mathbf{r}^*| = 1/|\mathbf{r}^*| \text{ as } h/h = \mathbf{a} \cdot \mathbf{a}^* = 1$$



The plane of the family (hkl) nearest to the origin.

The reciprocal lattice concept : 4

Some useful relationships (continued)

3. Weiss zone law

$$\mathbf{r}^* = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \text{ and } \mathbf{d} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

The plane (hkl) is in the zone [uvw] if \mathbf{r}^* is perpendicular to direction \mathbf{d} .

$$(h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) \cdot (u\mathbf{a} + v\mathbf{b} + w\mathbf{c}) = 0$$

$$hua^*.a + kvb^*.b + lwc^*.c = 0$$

$$\text{as } a^*.a = b^*.b = c^*.c = 1$$

$$hu + kv + lw = 0$$

Given two planes in the same zone (h1 k1 l1) and (h2 k2 l2)

Zone direction is $u:v:w = (k_1 l_2 - k_2 l_1) : (l_1 h_2 - l_2 h_1) : (h_1 k_2 - h_2 k_1)$

4. The angle "phi" between two planes (h1 k1 l1) and (h2 k2 l2)

$$\mathbf{r}_1^* = h_1\mathbf{a}^* + k_1\mathbf{b}^* + l_1\mathbf{c}^*$$

$$\mathbf{r}_2^* = h_2\mathbf{a}^* + k_2\mathbf{b}^* + l_2\mathbf{c}^*$$

$$\mathbf{r}_1^* \cdot \mathbf{r}_2^* = |\mathbf{r}_1^*| |\mathbf{r}_2^*| \cos(\phi)$$

$$\cos(\phi) = \mathbf{r}_1^* \cdot \mathbf{r}_2^* / |\mathbf{r}_1^*| |\mathbf{r}_2^*| = (h_1\mathbf{a}^* + k_1\mathbf{b}^* + l_1\mathbf{c}^*) \cdot (h_2\mathbf{a}^* + k_2\mathbf{b}^* + l_2\mathbf{c}^*) / (d_{h_1k_1l_1} d_{h_2k_2l_2})$$

$$d_{hkl} = 1 / |h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*|$$

$$d_{hkl} = 1 / \sqrt{(h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2klb^*c^*\cos(\alpha^*) + 2lhc^*a^*\cos(\beta^*) + 2hka^*b^*\cos(\gamma^*))}$$

Metric Tensor

- The metric tensor is useful to make crystallographic calculations on the direct lattice on any symmetry using matrix methods

- The metric tensor $M = \begin{bmatrix} \mathbf{a \cdot a} & \mathbf{a \cdot b} & \mathbf{a \cdot c} \\ \mathbf{b \cdot a} & \mathbf{b \cdot b} & \mathbf{b \cdot c} \\ \mathbf{c \cdot a} & \mathbf{c \cdot b} & \mathbf{c \cdot c} \end{bmatrix}$

Triclinic $\begin{bmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{bmatrix}$

Monoclinic $\begin{bmatrix} a^2 & 0 & ac \cos \beta \\ 0 & b^2 & 0 \\ ac \cos \beta & 0 & c^2 \end{bmatrix}$

Trigonal and hexagonal $\begin{bmatrix} a^2 & -\frac{1}{2}a^2 & 0 \\ -\frac{1}{2}a^2 & a^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}$

Orthorhombic $\begin{bmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}$

Tetragonal $\begin{bmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}$

Cubic $\begin{bmatrix} a^2 & 0 & 0 \\ 0 & a^2 & 0 \\ 0 & 0 & a^2 \end{bmatrix}$

Metric Tensor 2

- The scalar product of two directions is given by

$$[U_1 V_1 W_1] \begin{bmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{a} \cdot \mathbf{b} & \mathbf{a} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{b} \cdot \mathbf{c} \\ \mathbf{c} \cdot \mathbf{a} & \mathbf{c} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \end{bmatrix} \begin{bmatrix} U_2 \\ V_2 \\ W_2 \end{bmatrix}$$

This allows the calculation of the angle between

2 directions and the modulus of a direction

$$\cos(\text{angle}) = [UVW1] \cdot [UVW2] / |UVW1| |UVW2|$$

Reciprocal Metric Tensor

- In a similar way we can construct a reciprocal

metric tensor
$$\begin{bmatrix} \mathbf{a}^* \cdot \mathbf{a}^* & \mathbf{a}^* \cdot \mathbf{b}^* & \mathbf{a}^* \cdot \mathbf{c}^* \\ \mathbf{b}^* \cdot \mathbf{a}^* & \mathbf{b}^* \cdot \mathbf{b}^* & \mathbf{b}^* \cdot \mathbf{c}^* \\ \mathbf{c}^* \cdot \mathbf{a}^* & \mathbf{c}^* \cdot \mathbf{b}^* & \mathbf{c}^* \cdot \mathbf{c}^* \end{bmatrix}$$

Triclinic	$\begin{bmatrix} a^{*2} & a^*b^* \cos \gamma^* & a^*c^* \cos \beta^* \\ a^*b^* \cos \gamma^* & b^{*2} & b^*c^* \cos \alpha^* \\ a^*c^* \cos \beta^* & b^*c^* \cos \alpha^* & c^{*2} \end{bmatrix}$	Orthorhombic	$\begin{bmatrix} a^{*2} & 0 & 0 \\ 0 & b^{*2} & 0 \\ 0 & 0 & c^{*2} \end{bmatrix}$
Monoclinic	$\begin{bmatrix} a^{*2} & 0 & a^*c^* \cos \beta^* \\ 0 & b^{*2} & 0 \\ a^*c^* \cos \beta^* & 0 & c^{*2} \end{bmatrix}$	Tetragonal	$\begin{bmatrix} a^{*2} & 0 & 0 \\ 0 & a^{*2} & 0 \\ 0 & 0 & c^{*2} \end{bmatrix}$
Trigonal and hexagonal	$\begin{bmatrix} a^{*2} & \frac{1}{2}a^{*2} & 0 \\ \frac{1}{2}a^{*2} & a^{*2} & 0 \\ 0 & 0 & c^{*2} \end{bmatrix}$	Cubic	$\begin{bmatrix} a^{*2} & 0 & 0 \\ 0 & a^{*2} & 0 \\ 0 & 0 & a^{*2} \end{bmatrix}$

- $\cos(\text{angle}) = [\mathbf{hkl1}] \cdot [\mathbf{hkl2}] / |\mathbf{hkl1}| |\mathbf{hkl2}|$

Using reciprocal metric tensor

The crystal direction $[u \ v \ w]$ normal to the plane $(h \ k \ l)$ is given by

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} \mathbf{a}_1^* \cdot \mathbf{a}_1^* & \mathbf{a}_1^* \cdot \mathbf{a}_2^* & \mathbf{a}_1^* \cdot \mathbf{a}_3^* \\ \mathbf{a}_2^* \cdot \mathbf{a}_1^* & \mathbf{a}_2^* \cdot \mathbf{a}_2^* & \mathbf{a}_2^* \cdot \mathbf{a}_3^* \\ \mathbf{a}_3^* \cdot \mathbf{a}_1^* & \mathbf{a}_3^* \cdot \mathbf{a}_2^* & \mathbf{a}_3^* \cdot \mathbf{a}_3^* \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix}$$

Crystallographic to orthogonal axes

- Many calculations are simple and more familiar in a orthogonal or Cartesian basis
- A transformation matrix (CO) crystal to orthogonal.

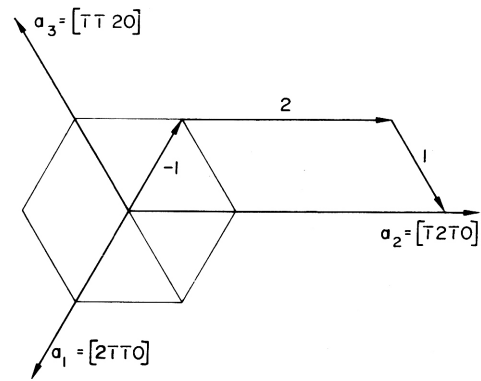
$$\begin{pmatrix} a_0 \sin \beta & b_0 u & 0 \\ 0 & b_0 v & 0 \\ a_0 \cos \beta & b_0 \cos \alpha & c_0 \end{pmatrix}$$

where

$$u = \frac{\cos \gamma - \cos \alpha \cos \beta}{\sin \beta} \quad \text{and} \quad v = \sqrt{\sin^2 \alpha - u^2}$$

- $V_{\text{orthogonal}} = \text{CO} \cdot V_{\text{crystal-uvw}}$
- $V_{\text{orthogonal}} = \text{transpose}(\text{CO}^{-1}) \cdot V_{\text{crystal-hkl}}$
- $V_{\text{crystal-uvw}} = \text{transpose}(\text{CO}^{-1}) \cdot V_{\text{orthogonal}}$
- $V_{\text{crystal-hkl}} = \text{CO} \cdot V_{\text{orthogonal}}$

Direction [uvtw]



Determination of direction indices in the basal plane of a hexagonal crystal.

[UVW] and [uvw] in hexagonal axes

For these two vectors to be identical

$$U\mathbf{a} + V\mathbf{b} + W\mathbf{c} = u\mathbf{a} + v\mathbf{b} + t\mathbf{d} + w\mathbf{c}$$

Since the x, y, and u axes are inclined at 120° to one another and $a = b = d$,

$$\mathbf{a} + \mathbf{b} + \mathbf{d} = 0$$

Hence $U\mathbf{a} + V\mathbf{b} + W\mathbf{c} = (u-t)\mathbf{a} + (v-t)\mathbf{b} + w\mathbf{c}$

and $U = u - t$

$$V = v - t$$

$$W = w$$

These equations are adequate to convert Weber symbols to Millerian zone axis symbols, but to convert in the opposite direction it is necessary to apply the condition

$$u + v + t = 0$$

whence $U = 2u + v$

$$V = u + 2v$$

$$W = w$$

so that $u = \frac{2U - V}{3}$

$$v = \frac{2V - U}{3}$$

$$t = -\frac{U + V}{3}$$

$$w = W.$$

The condition for the plane (*hkl*) to lie in the zone [UVW] is $hU + kV + lW = 0$, which becomes when the equivalent Weber symbol [uvw] is used

$$h(u-t) + k(v-t) + lw = 0$$

i.e. $hu + kv - (h+k)t + lw = 0$.

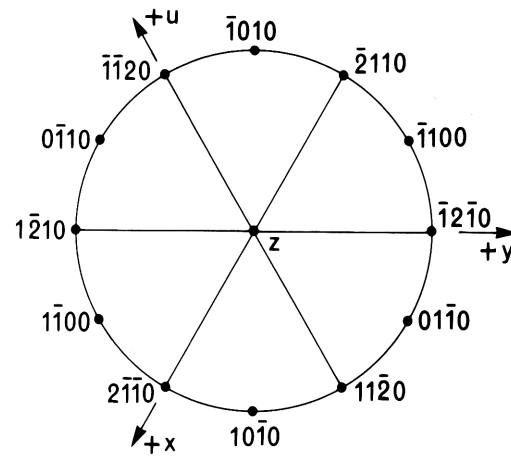
And if the Miller-Bravais index *i* is introduced, where $h + k + i = 0$, this equation becomes

$$hu + kv + it + lw = 0,$$

the condition for the plane (*hkil*) to lie in the zone [uvw]. For example the zone $[\bar{1}\bar{2}\bar{1}3]$ contains the planes $(10\bar{1}0)$, $(0\bar{1}11)$, $(1\bar{2}12)$ and the zone $[0\bar{1}11]$ contains the planes $(2\bar{1}\bar{1}0)$, $(10\bar{1}1)$, $(11\bar{2}3)$.

Planes (hkil)

$$h+k+i = 0$$

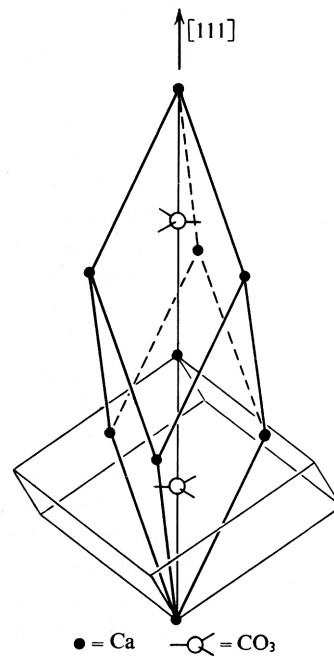


Stereogram of the forms $\{10\bar{T}0\}$ and $\{11\bar{T}0\}$ in point group 6 illustrate Miller-Bravais indexing.

Comparison of Miller-Bravais indices and Miller indices of the forms $\{10\bar{T}0\}$ and $\{11\bar{T}0\}$

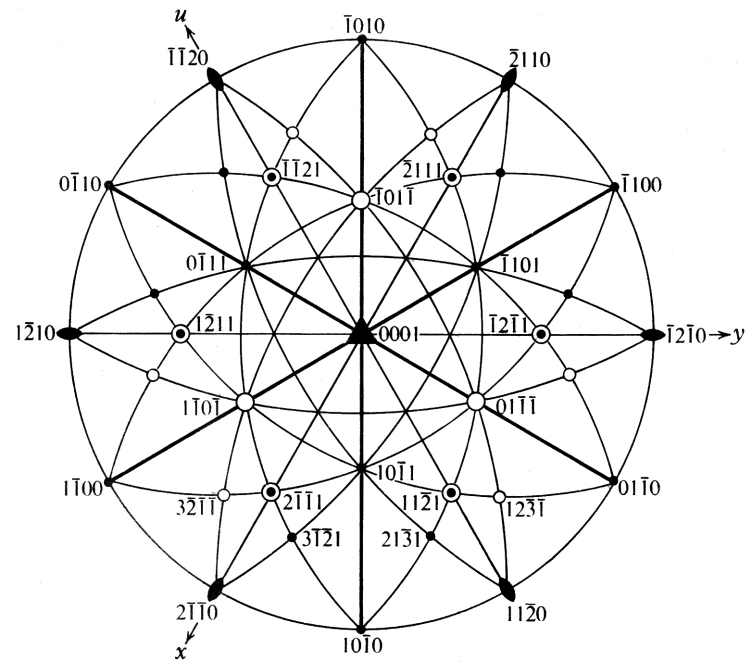
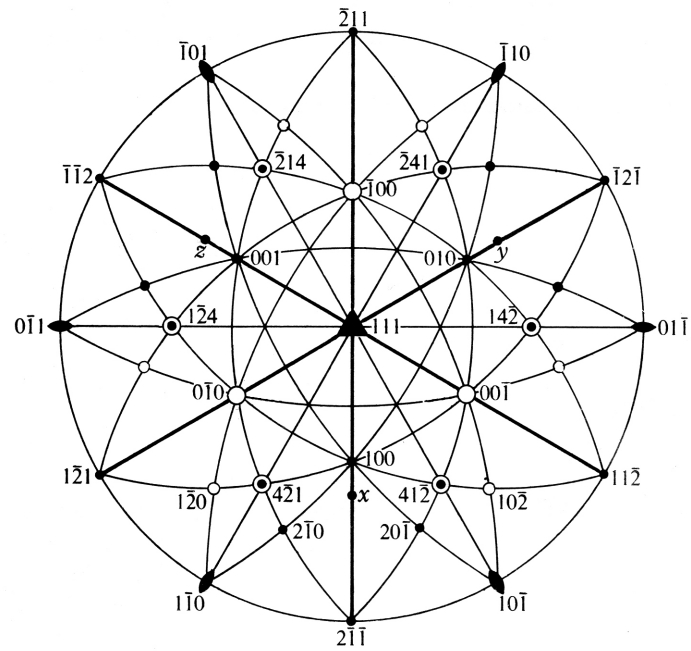
Miller-Bravais	Miller	Miller-Bravais	Miller
$(10\bar{T}0)$	(100)	$(2\bar{T}\bar{T}0)$	$(2\bar{T}0)$
$(01\bar{T}0)$	(010)	$(11\bar{T}0)$	(110)
$(\bar{T}100)$	$(\bar{T}10)$	$(\bar{T}2\bar{T}0)$	$(\bar{T}20)$
$(\bar{T}010)$	$(\bar{T}00)$	$(\bar{T}210)$	$(\bar{T}210)$
$(0\bar{T}10)$	$(0\bar{T}0)$	$(\bar{T}\bar{T}20)$	$(\bar{T}\bar{T}0)$
$(1\bar{T}00)$	$(1\bar{T}0)$	$(1\bar{T}20)$	$(1\bar{T}0)$

'Cleavage' and Rhombohedral cells

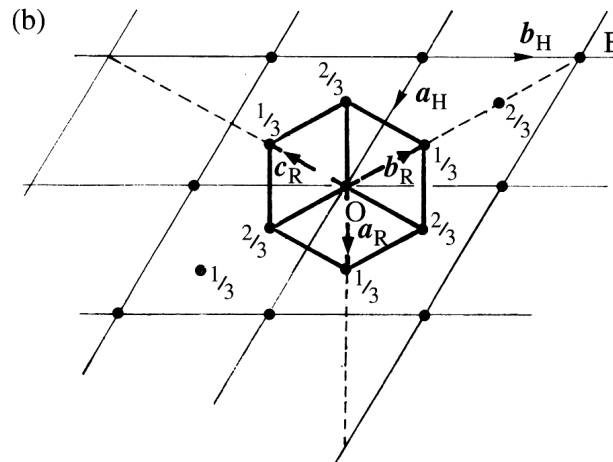
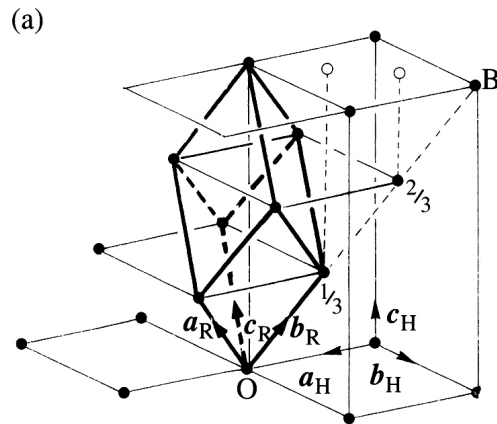


The structure of calcite (CaCO₃). The primitive rhombohedral unit cell is shown which contains two formula units of CaCO₃. The cell outlined with weak lines is the smallest 'cleavage rhombohedron' and contains four units of CaCO₃.

Rhombhedral and hexagonal axes

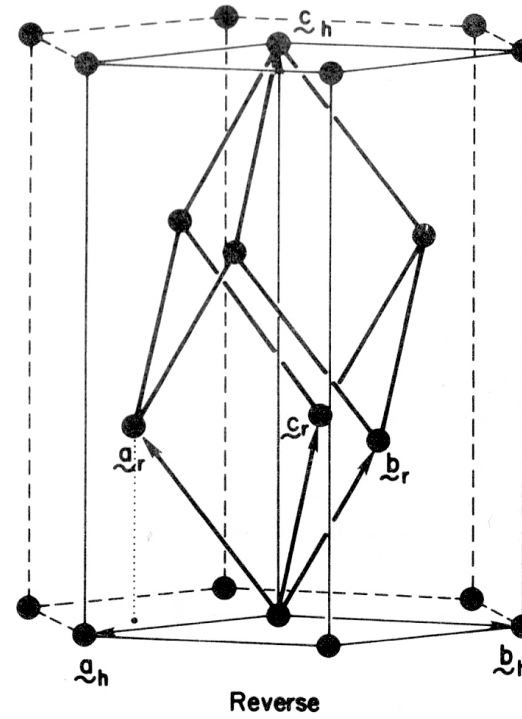
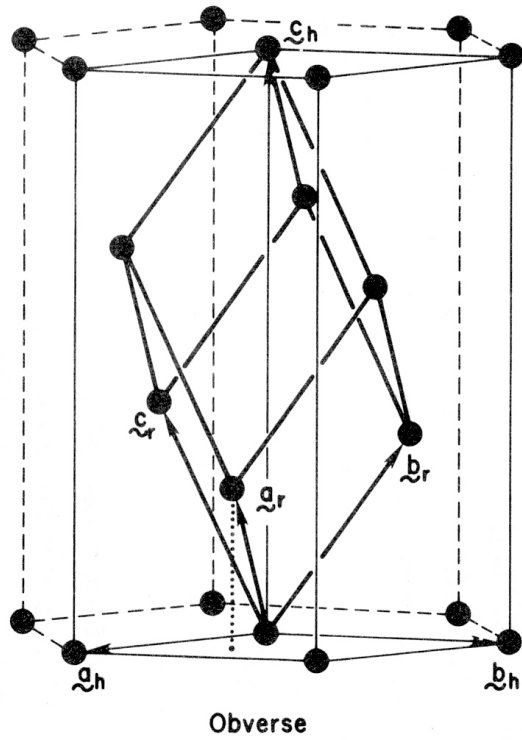


Rhombohedral and hexagonal cell

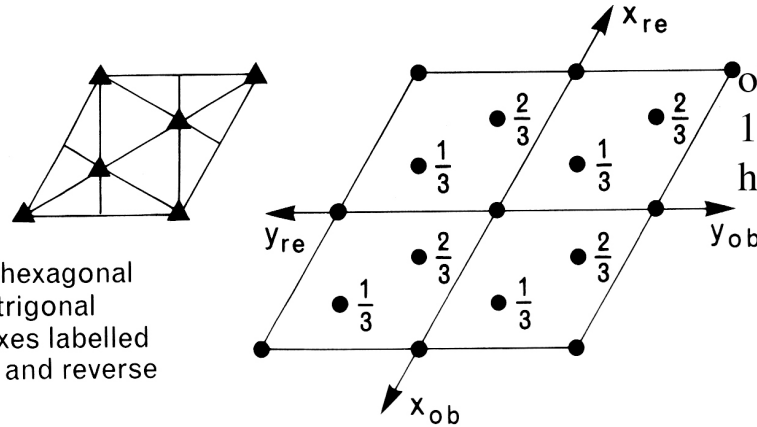


Rhombohedral lattice. The basis of the rhombohedral cell is labelled a_R , b_R , c_R , the basis of the hexagonal centred cell is labelled a_H , b_H , c_H (numerical fractions are calculated in terms of the c_H axis). (a) Obverse setting; (b) the same figure as in (a) projected along c_H .

Obverse and Reverse Rhombhedral cells

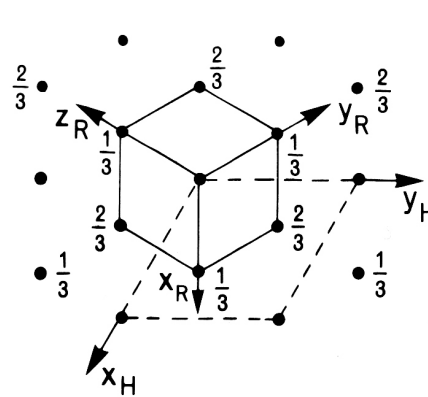


Obverse and Reverse on hexagonal axes

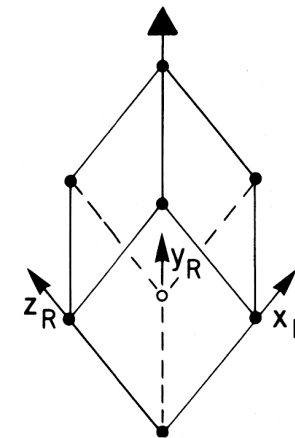


obverse to reverse
180° rotation in
hexagonal cell

The triple hexagonal unit-cell of the trigonal R-lattice with axes labelled for the obverse and reverse orientations.



The relationship between the rhombohedral and triple hexagonal unit-cells for the trigonal R-lattice; the right hand diagram shows the rhombohedral unit-cell in perspective.



The rhombohedral Bravais lattice