Fundamentals of Fourier transform

International School on Fundamental Crystallography with applications to Electron Crystallography
June 27 - July 2, 2016 - University of Antwerp

Based on “Transform methods in crystallography”, by Jan C. J. Bart
Periodic functions

A Fourier series decomposes any **periodic** function into the sum of a (possibly infinite) set of simple oscillating functions, (sines and cosines or complex exponentials).

\[ f(x) \text{ is a periodic function of a real variable } x \text{ with period } P \text{ if:} \]

\[ f(x+P) = f(x) \]
Fourier series

Let \( f(x) \) be a periodic function integrable on the interval \((x_0, x_0 + P)\), where \( P \) is the period. We can represent \( f \) in that interval by a series of sinusoidal functions:

\[
f_N(x) = \frac{A_0}{2} + \sum_{n=1}^{N} A_n \sin \left( \frac{2\pi nx}{P} + \varphi_n \right), \quad N \geq 1
\]

\( f_N(x) \) approximates \( f(x) \) \([x_0, x_0 + P]\), and the approximation improves as \( N \to \infty \). The infinite sum, \( f_\infty(x) \), is called the \textbf{Fourier series} representation of \( f(x) \).
Fourier series

\[
\frac{4 \sin \theta}{\pi}
\]

\[
\frac{4 \sin 3\theta}{3\pi}
\]

\[
\frac{4 \sin 5\theta}{5\pi}
\]

\[
\frac{4 \sin 7\theta}{7\pi}
\]
Integral transforms

The integral transform of a function $f(x)$ is defined as:

$$F(k) = \int_a^b K(k, x) f(x) \, dx$$

where $K(k, x)$ is a function of both $k$ and $x$ and is called the kernel of the transform. $k$ and $x$ represent variables (or vectors of variables) in two dual spaces and the transform realizes the “tunnel” between the two spaces.

Depending of the kernel, we have different types of integral transforms.
Integral transforms

Laplace transform:

\[ F(k) = \int_{0}^{\infty} e^{-kx} f(x) \, dx \]

Fourier transform:

\[ F(k) = \int_{-\infty}^{\infty} e^{\pm ikx} f(x) \, dx \]

Hankel transform:

\[ F(k) = \int_{0}^{\infty} J_n(kx) f(x) \, dx \]

\( J_n \): Bessel function of order \( n \)
Fourier transform

If \( f(x) \) is a function of \( x \) such that:

\[
\int_{-\infty}^{\infty} \left| f(x) \right|^2 \, dx
\]

is finite, then:

\[
F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx = \mathcal{T} \left[ f(x) \right]
\]

\[
f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} \, dk = \mathcal{T}^{-1} \left[ F(k) \right]
\]
Fourier transform

\[ F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx = A(k) - iB(k) \]

\[ A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \cos(kx) \, dx \]

\[ B(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \sin(kx) \, dx \]

\[ f(x) = f(-x) \Rightarrow F(k) = A(k) \in \mathbb{R} \]

\[ f(x) = -f(-x) \Rightarrow F(k) = -iB(k) \in \mathbb{C} \]
A step function of a real variable $x$ is a function which changes its value only on a discrete set of discontinuities. The function values at the discontinuities may or may not be defined.
The **Heaviside step function** $H(x)$ (or **unit step function**) is a discontinuous function whose value is zero for negative argument and one for positive argument.
A boxcar function is any function which is zero over the entire real line except for a single interval where it is equal to a constant, $A$.

$$f(x) = A \cdot [H(x-a) - H(x-b)]$$
Fourier transform of the boxcar function

F(k) = Al \cdot \sin(\pi lk) / \pi lk

Fraunhofer diffraction amplitude of a slit of width 2\pi l

The widths of f(x) and F(k) are inversely proportional
Diffraction of light occurs when a beam of light is partly blocked by an obstacle and some of the light is scattered around the object; light and dark bands are often seen at the edge of the shadow.

If both the light source and the viewing plane are at infinity with respect to the diffracting aperture, the incident light is a plane wave, the phase of the light at each point in the aperture is the same.

Concretely, Fraunhofer diffraction occurs for the “far field condition”:

\[ W^2 \ll L\lambda \]

\( W \): aperture size; \( L \): distance from the aperture; \( \lambda \): wavelength
Single-slit diffraction

A long slit of infinitesimal width which is illuminated by light diffracts the light into a series of circular waves and the wavefront which emerges from the slit is a cylindrical wave of uniform intensity. A slit which is wider than a wavelength produces interference effects in the space downstream of the slit.

slit of width equal to wavelength

slit of width equal to five times the wavelength
The Dirac delta function, or $\delta$ function, is a distribution on the real number line that is zero everywhere except at zero, with an integral of one over the entire real line and can be seen as as the limit of the sequence of zero-centred normal (Gaussian) distributions.

Gaussian function $\delta_p(x) = \sqrt{\frac{p}{\pi}} \exp(-px^2)$

Dirac delta $\delta \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \end{cases}$
A convolution is an integral that expresses the amount of overlap of one function $g$ as it is shifted over another function $f$. It is defined as the integral of the product of the two functions after one is reversed and shifted.

$$f(t) * g(t) = \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d\tau = \int_{-\infty}^{\infty} f(t-\tau)g(\tau)d\tau$$

- the origin of the function $f$ is set in every position of the function $g$
- the value of $f$ in each position is multiplied by the value of $g$ at that point
- the sum is taken over all possible points
The convolution of a function $f(x)$ with a delta function $\delta(x - x_0)$ gives the function $f(x_0)$. 
Fourier transform of convolutions

\[ F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx = \mathcal{T}[f(x)] \]

\[ G(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x) e^{-ikx} \, dx = \mathcal{T}[g(x)] \]

\[ \mathcal{T}[f(x) \ast g(x)] = \mathcal{T}[f(x)] \cdot \mathcal{T}[g(x)] \]
Tunnelling dual spaces

Space 1 (direct space)

- Summation: $f(x) + g(x)$
- Multiplication: $f(x) \cdot g(x)$
- Convolution: $f(x) \ast g(x)$

Space 2 (reciprocal space)

- Summation: $\mathcal{T}[f(x)] + \mathcal{T}[g(x)]$
- Convolution: $\mathcal{T}[f(x)] \ast \mathcal{T}[g(x)]$
- Multiplication: $\mathcal{T}[f(x)] \cdot \mathcal{T}[g(x)]$
A Dirac comb (impulse train, sampling function) is an infinite series of Dirac delta functions spaced at intervals of $T$

$$C_T(t) = \sum_{k=-\infty}^{\infty} \delta(t - kT)$$
Fourier transform of a Dirac delta

\[ \mathcal{T} \left[ \delta(x) \right] = \int_{-\infty}^{\infty} e^{-2\pi i k x} \delta(x) \, dx = 1 \]
Two different ways of addressing the problem of diffraction by a crystal
• the **classical theory** introduces first the lattice (periodic object) and later the scattering matter
• the **Fourier transform theory** follows the inverse route and first considers the unit-cell content (non-periodic object) and then examines how the diffraction pattern is modified by forming a regular array of cells.
The Fourier expansion of a continuous *periodic* distribution $\rho(\mathbf{r})$ (*classical theory*) is given by the Fourier series:

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{H}} F(\mathbf{H}) \exp(-2\pi i \mathbf{H} \cdot \mathbf{r})$$

$$F(\mathbf{H}) = \sum_{j=1}^{N} f_j(\mathbf{H}) \exp(2\pi i \mathbf{H} \cdot \mathbf{r}_j)$$

In the Fourier transform theory we consider a *non-periodic* electron distribution $\rho(\mathbf{r})$. The discrete vector $\mathbf{H}$, pointing to the reciprocal lattice nodes, is replaced by a continuous vector $\mathbf{r}^*$ which may end at any point of the reciprocal space. The equations used in the classical theory are modified accordingly:

$$\rho(\mathbf{r}) = \int_{\mathbf{r}^*} F(\mathbf{r}^*) \exp(-2\pi i \mathbf{r}^* \cdot \mathbf{r}) dV_{\mathbf{r}^*}$$

$$F(\mathbf{r}^*) = \int_{V_{\mathbf{r}}} \rho(\mathbf{r}) \exp(2\pi i \mathbf{r}^* \cdot \mathbf{r}) dV_{\mathbf{r}}$$
Diffraction by non-periodic objects

Discontinuous medium

$N$ point scatterers ($\delta$ functions of weight $a_j$) at positions $r_j$

$$F(r^*) = \sum_{j=1}^{N} a_j \exp(2\pi i r^* \cdot r_j)$$

N.B. $a_j$ is not a function of $r^*$

Continuous medium

$$F(r^*) = \int \rho(r) \exp(2\pi i r^* \cdot r) dV_r$$

The wave scattered by a continuous medium can be represented as the Fourier transform of the scattering density $\rho(r)$, for all coherent scattering processes (optical, X-rays, neutrons, electrons)
Fourier transform of the electron density in an atom

\[ f(r^*) = \int_{\text{atom}} \rho(r) \exp(2\pi i r^* \cdot r) dV_r. \]

\( \rho(r) \): electron density distribution of the atom at rest
\( f(r^*) \): atomic scattering factor

**Vibrating atom**

- The time of a diffraction experiment is much longer than the time of the atomic vibrations
- Approximation: the vibration of an atom is independent from that of its neighbours

\( p(r_1) \): probability that the centre of an atom be at position \( r_1 \)
\( \rho_a(r) \): electron density of the atom at equilibrium in \( r \)
\( \rho_a^v(r) \): electron density of the atom vibrating around the position \( r \)
Fourier transform of the electron density in an atom

\[ \rho_a^v(r) = \int \rho(r - r_1) p(r_1) \, dr_1 = \rho_a(r) \ast p(r) \]

Scattering factor for the vibrating atom

\[ f_a^v(r*) = \mathcal{T}^{-1} \left[ \rho_a^v(r) \right] = \mathcal{T}^{-1} \left[ \rho_a(r) \ast p(r) \right] = f_a(r*) \cdot q(r*) \]

- \( f_a^v(r) \): scattering factor of the vibrating atom
- \( f_a(r) \): scattering factor of the atom at rest
- \( q(r*) \): atomic displacement factor (Debye-Waller factor)
Fourier transform of the electron density in an atom

**Harmonic vibration**

\[ q(\mathbf{r}^*) = \exp(-\mathbf{r}^* \cdot \mathbf{B} \mathbf{r}^*) \]

\( \mathbf{B} \): second rank tensor describing an ellipsoid

**Isotropic (spherical) vibration**

\( \mathbf{B} = \mathbf{B} \mathbf{I} \) (\( \mathbf{I} \) = identity matrix, \( B = \text{constant} \))

\[ q(\mathbf{r}^*) = \exp(-B\mathbf{r}^* \cdot \mathbf{I} \mathbf{r}^*) = \exp(-B |\mathbf{r}^*|^2) = \exp\left(-B \frac{1}{d_{hkl}^2}\right) \]

\[ \lambda = 2d_{hkl} \sin \theta_{hkl} \]

\[ q(\mathbf{r}^*) = \exp\left(-B \frac{\sin^2 \theta_{hkl}}{\lambda^2}\right) \]
Effect of translation of Fourier transform

\[ \rho_T(r) = \rho(r-t) \quad t = \text{translation vector} \quad F_T(r^*) = T^{-1}[\rho_T(r)] \]

\[ F_T(r^*) = \int \rho(r - t) \exp(2\pi ir^* \cdot r) dV_r = \]

\[ = \exp(2\pi ir^* \cdot t) \int \rho(r - t) \exp(2\pi ir^* \cdot r - t) dV_r = \]

\[ = F(r^*) \exp(2\pi ir^* \cdot t) \]

Translation of \( \rho(r) \) by a vector \( t \) in direct space is equivalent to modifying the Fourier transform by the phase factor \( \exp(2\pi ir^* \cdot t) \) in reciprocal space, without change in the modulus \( |F(r^*)| \), but the real and imaginary part of \( F(r^*) \) are multiplied by \( \cos(2\pi r^* \cdot t) \) and \( \sin(2\pi r^* \cdot t) \) respectively. A description of a transform is thus \textit{origin dependent}.

The Fourier transform of a centrosymmetric body is real only if the origin is taken at the centre of symmetry (\textit{origin choice 2} of the \textit{International Tables for Crystallography}).
$\mathbf{r}_j$: vector specifying the position of the j-th atom with respect to an arbitrary origin

$f_j(\mathbf{r}^*)$: Fourier transform of the j-th atom referred to its centre as origin

**Fourier transform of a set of atoms**

$$F_T(\mathbf{r}^*) = F(\mathbf{r}^*) \exp(2\pi i \mathbf{r}^* \cdot \mathbf{t})$$

$$F(\mathbf{r}^*) = \sum_{j=1}^{N} f_j(\mathbf{r}^*) \exp\left(2\pi i \mathbf{r}^* \cdot \mathbf{r}_j\right)$$

$f_j$ is a function of $\mathbf{r}^*$ (it was not the case for point scatterers)

For spherically symmetrical atoms $f_j(\mathbf{r}^*) = f_j(\mathbf{r}^*)$ and $f_j$ varies as a function of $r^* = |\mathbf{r}^*| = 2\sin\vartheta/\lambda$, due to its finite size (not point scatterer).
Fourier transform of a finite lattice

**lattice vectors:** \( \mathbf{r}(u,v,w) = u\mathbf{a} + v\mathbf{b} + w\mathbf{c} \)

Set of delta functions with weight \( f_j \) at lattice nodes

\[
f_L(\mathbf{r}) = \sum_j f_j \delta(\mathbf{r} - \mathbf{r}_j) = \sum_{u,v,w} f(uvw) \delta(\mathbf{r} - u\mathbf{a} + v\mathbf{b} + w\mathbf{c})
\]

Point scatterers

\[
F(\mathbf{r}^*) = \sum_{j=1}^{N} a_j \exp(2\pi i \mathbf{r}^* \cdot \mathbf{r}_j)
\]

Fourier transform of a set of delta functions with weight \( f_j \)

Lattice (\( f_j = 1 \))

\[
F_L(\mathbf{r}^*) = \sum_{u,v,w} \exp\left[2\pi i \mathbf{r}^* \cdot (u\mathbf{a} + v\mathbf{b} + w\mathbf{c})\right]
\]
Fourier transform of a finite lattice

\[ F_L(\mathbf{r}^\ast) = \sum_u \exp(2\pi i u \mathbf{r^\ast} \cdot \mathbf{a}) \sum_v \exp(2\pi i v \mathbf{r^\ast} \cdot \mathbf{b}) \sum_w \exp(2\pi i w \mathbf{r^\ast} \cdot \mathbf{c}) \]

\[ F_L(\mathbf{r}^\ast) = \frac{\sin N_1 \pi \mathbf{a} \cdot \mathbf{r^\ast}}{\sin \pi \mathbf{a} \cdot \mathbf{r^\ast}} \cdot \frac{\sin N_2 \pi \mathbf{b} \cdot \mathbf{r^\ast}}{\sin \pi \mathbf{b} \cdot \mathbf{r^\ast}} \cdot \frac{\sin N_3 \pi \mathbf{c} \cdot \mathbf{r^\ast}}{\sin \pi \mathbf{c} \cdot \mathbf{r^\ast}} \]

\(N_1, N_2, N_3\): number of equally spaced delta functions along \(\mathbf{a}^\ast, \mathbf{b}^\ast, \mathbf{c}^\ast\)

The maxima of \(F_L(\mathbf{r^\ast})\) correspond to the conditions:

\[ \mathbf{r^\ast} \cdot \mathbf{a} = h \in \mathbb{Z} \]

\[ \mathbf{r^\ast} \cdot \mathbf{b} = k \in \mathbb{Z} \]

\[ \mathbf{r^\ast} \cdot \mathbf{c} = l \in \mathbb{Z} \]
Fourier transform of an infinite lattice

\[ F_L (\mathbf{r}^*) = \sum_{u,v,w=-\infty}^{\infty} \exp \left[ 2\pi i \mathbf{r}^* \cdot (u \mathbf{a} + v \mathbf{b} + w \mathbf{c}) \right] \]

\[ F_L (\mathbf{r}^*) = \sum_{u=-\infty}^{\infty} \exp (2\pi i u r^* \cdot \mathbf{a}) \sum_{v=-\infty}^{\infty} \exp (2\pi i v r^* \cdot \mathbf{b}) \sum_{w=-\infty}^{\infty} \exp (2\pi i w r^* \cdot \mathbf{c}) \]

\[ F_L (\mathbf{r}^*) = \lim_{N_1,N_2,N_3 \to \infty} \frac{\sin N_1 \pi \mathbf{a} \cdot \mathbf{r}^*}{\sin \pi \mathbf{a} \cdot \mathbf{r}^*} \cdot \frac{\sin N_2 \pi \mathbf{b} \cdot \mathbf{r}^*}{\sin \pi \mathbf{b} \cdot \mathbf{r}^*} \cdot \frac{\sin N_3 \pi \mathbf{c} \cdot \mathbf{r}^*}{\sin \pi \mathbf{c} \cdot \mathbf{r}^*} \]

\( F_L (\mathbf{r}^*) \) is non-zero only when:

\[ \mathbf{r}^* \cdot \mathbf{a} = h \in \mathbb{Z} \quad \mathbf{r}^* \cdot \mathbf{b} = k \in \mathbb{Z} \quad \mathbf{r}^* \cdot \mathbf{c} = l \in \mathbb{Z} \]

\[ F_L (\mathbf{r}^*) = \frac{1}{V} \sum_{h,k,l=-\infty}^{\infty} \delta (\mathbf{r}^* - \mathbf{r}_{hkl}^*) \]

The \textit{discrete} vector \( \mathbf{r}_{hkl}^* \) defines the \textit{reciprocal lattice}. 
A crystal (periodic structure) is described as consisting of two functions: 
1. the real (direct) lattice function \( f_L(\mathbf{r}) \), which is unity at each lattice node and zero elsewhere: 
2. the electron density function \( \rho(\mathbf{r}) \), describing the content of a unit cell.

The content of the crystal is the convolution of the periodic function \( f_L(\mathbf{r}) \) and the finite function \( \rho(\mathbf{r}) \)

\[
\hat{f}_C(\mathbf{r}) = \hat{f}_L(\mathbf{r}) \ast \rho(\mathbf{r})
\]

The Fourier transform of the content of the crystal is the product of the Fourier transforms of the lattice and of the unit cell content

\[
F_C(\mathbf{r}^*) = F_L(\mathbf{r}^*) \cdot F(\mathbf{r}^*)
\]

\[
F_L(\mathbf{r}^*) = \frac{1}{V} \sum_{h,k,l=-\infty}^{\infty} \delta(\mathbf{r}^* - \mathbf{r}^*_{hkl})
\]

\[
F(\mathbf{r}_{hkl}^*) = \sum_{j=1}^{N} f_j(\mathbf{r}^*) \exp \left( 2\pi i \mathbf{r}^* \cdot \mathbf{r}_j \right)
\]
Fourier transform of the content of the crystal

\[ F_C(\mathbf{r}^*) = F_L(\mathbf{r}^*) \cdot F(\mathbf{r}^*) \]

\[ F_L(\mathbf{r}^*) = \frac{1}{V} \sum_{h,k,l=-\infty}^{\infty} \delta(\mathbf{r}^* - \mathbf{r}_{hkl}^*) \]

\[ F(\mathbf{r}^*) = \sum_{j=1}^{N} f_j(\mathbf{r}^*) \exp(2\pi i \mathbf{r}^* \cdot \mathbf{r}_j) \]

\[ \int F(\mathbf{r}^*) \delta(\mathbf{r}^* - \mathbf{r}_{hkl}^*) dV_{\mathbf{r}^*} = F(\mathbf{r}_{hkl}^*) = \]

\[ = \sum_{j=1}^{N} f_j(\mathbf{r}_{hkl}^*) \exp(2\pi i \mathbf{r}_{hkl}^* \cdot \mathbf{r}_j) \]
A note on domain structures

\[ F_T(\mathbf{r}^*) = F(\mathbf{r}^*) \exp(2\pi i \mathbf{r}^* \cdot \mathbf{t}) \]

\( I(hkl) \propto |F(hkl)|^2 \)

**Twin domains**
(differing by orientation)
Visible in the diffraction pattern

**Antiphase domains**
(differing by position)
Invisible in the diffraction pattern
(effect on the *phase*)
Visible by electron microscopy

**G** group of the parent phase

**H** group of the daughter phase

*translationengleiche* subgroup
(same lattice, lower point group)

*klassengleiche* subgroup
(sublattice, same point group)

\( r \in \mathbb{R}^3 \)
Fundamentals. Crystal patterns and crystal structures. Lattices, their symmetry and related basic concepts

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Ideal vs. real crystal, perfect vs. imperfect crystal

Ideal crystal:
Perfect periodicity, no static (vacancies, dislocations, chemical heterogeneities, even the surface!) or dynamic (phonons) defects.

Real crystal:
A crystal whose structure differs from that of an ideal crystal for the presence of static or dynamic defects.

Perfect crystal:
A real crystal whose structure contains only equilibrium defects.

Imperfect crystal:
A real crystal whose structure contains also non-equilibrium defects (dislocations, chemical heterogeneities...).

What follows describes the structure of an ideal crystals (something that does not exist!), whereas *a real crystal is rarely in thermodynamic equilibrium.*
What do you get from a (conventional) diffraction experiment?

**Time and space averaged structure!**

“**Time-averaged**” because the time span of a diffraction experiment is much larger than the time of an atomic vibration.

The instantaneous position of an atom is replaced by the envelop (most often an ellipsoid) that describes the volume spanned by the atom during its vibration.

“**Space-averaged**” because a conventional diffraction experiment gives the average of the atomic position in the whole crystal volume, which corresponds to “the” position of the atom only if perfect periodicity is respected.

**Importance of studying the “ideal” crystal**

Non-conventional experiments (time-resolved crystallography, nanocrystallography etc.) allow to go beyond the ideal crystal model, but also some information that are often neglected in a conventional experiment (diffuse scattering) can give precious insights on the real structure of the crystal under investigation.
Transformations

Affine transformation

Euclidean transformation or isometry

Symmetry operation
A crystal pattern is an idealized crystal structure which makes abstraction of the defects (including the surface!) and of the atomic nature of the structure. A crystal pattern is therefore infinite and perfect. A crystal pattern is perfectly periodic and symmetric: periodicity affects symmetry and symmetry affects periodicity. A crystal pattern has both translational symmetry and point symmetry; these are described by its space group. We have to define the concepts of group and its declinations in crystallography.
Crystal structure/pattern vs. crystal lattice

- Crystal
- Molecule or coordination polyhedron
- Crystal pattern (crystal structure)
- Unit cell
- Lattice nodes
- Translations
The minimal unit you need to describe a crystal pattern

Asymmetric unit*

Unit cell

*In mathematics, it is called “fundamental region”
The concepts of chirality and handedness (the left-right difference)

Symmetry operations are classified into **first kind** (keep the handedness) and **second kind** (change the handedness).
If the object on which the operation is applied is non-chiral, the effect of the operation on the handedness is not visible but the **nature of the operation** (first or second kind) is not affected!

The **determinant** of the matrix representation of a symmetry operation is +1 (first kind) or -1 (second kind)
A symmetry group \((G, \circ)\) is a set \(G\) with a binary operation \(\circ\) having the following features:

- the elements of the set are symmetry operations;
- the binary operation \(\circ\) is a successive application of two symmetry operations \(g_i\) and \(g_j\) of the set \(G\), which gives as a result a symmetry operation \(g_k\) of the same set \(G\) (closure property):
  \[ g_i \in G \circ g_j \in G \rightarrow g_k \in G \quad (g_i \circ g_j = g_k) \]
- the binary operation is associative:
  \[ g_i (g_j \circ g_k) = (g_i \circ g_j) g_k \]
- the set \(G\) includes the identity (left and right identical):
  \[ e g_i = g_i e \]
- for each element of the set \(G\) (each symmetry operation) the inverse element (inverse symmetry operation) is in the set \(G\):
  \[ g_i^{-1} g_i = g_i g_i^{-1} = e \]

In the following we will normally speak of a group \(G\): it is a shortened expression for group \((G, \circ)\) where \(\circ\) is the successive application. Rigorously speaking, \(G\) is not a group but just a set!
The notion of “order”

**Order of a group element:** the smallest \( n \) such that \( g^n = e \)

**Order of a group:** the number of elements of the group (finite or infinite)

A special case of Abelian groups: cyclic groups

A **cyclic group** is a special Abelian group in which all elements of the group are generated from a single element (the generator).

\[
G = \{g, g^2, g^3, \ldots, g^n = e\}
\]

If \( n = \infty \) the group is infinite

A cyclic group is Abelian

\[
g^n g^m (n = m+p) = g^{m+p} g^m = (g^m g^p) g^m = g^m (g^p g^m) = g^m g^{p+m} = g^n g^n
\]
A note of nomenclature

• The *elements* of the group \((G, \circ)\) are *operations*
• The *operations* are performed about *geometric elements*
• A geometric element together with the set of symmetry operations performed about it is called a *symmetry element*
One-dimensional lattices

Symmetry operations

Identity
Translations
Reflections

How many 1D lattices are there? **Infinite!**

etc. etc.

How many *types of* 1D lattice are there? **One**
Coordinates of lattice nodes, direction indices $[uv]$
Symmetry in $E^2$

Operations that leave invariant all the space (2D): the identity
Operations that leave invariant one direction of the space (1D): reflections
Operations that leave invariant one point of the space (0D): rotations
Operations that do not leave invariant any point of the space: translations

The subspace left invariant (if any) by the symmetry operation has dimensions from 0 to $N$ (= 2 here)

Two independent directions in $E^2 \Rightarrow$ two axes ($a$, $b$) and one interaxial angle ($\gamma$)
## Types of symmetry elements and operations in E² (Hermann-Mauguin symbols)

### Operations of the first kind (no change of chirality)

<table>
<thead>
<tr>
<th>Element</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rotation point</td>
<td>Rotation</td>
</tr>
<tr>
<td>1</td>
<td>2π/1</td>
</tr>
<tr>
<td>2</td>
<td>2π/2</td>
</tr>
<tr>
<td>3</td>
<td>2π/3</td>
</tr>
<tr>
<td>4</td>
<td>2π/4</td>
</tr>
<tr>
<td>6</td>
<td>2π/6</td>
</tr>
</tbody>
</table>

### Operations of the second kind (change of chirality)

<table>
<thead>
<tr>
<th>Element</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reflection line</td>
<td>(mirror)</td>
</tr>
<tr>
<td>( m )</td>
<td></td>
</tr>
</tbody>
</table>

*Operations obtained as combination with a translation are introduced later*

The orientation in space of a reflection line is always expressed with respect to the lattice direction to which it is perpendicular.
Choice of the unit cell

primitive \((p)\) cells

centred \((c)\) cell
A lattice (infinite) can be represented by many different (finite) unit cells. 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**.
Conventional cell parameters and symmetry directions in the four crystal families of E²

**Monoclinic**
- No restriction on \( a, b, \gamma \)
- No symmetry direction

**Orthorhombic**
- No restriction on \( a, b \)
- \( \gamma = 90^\circ \)
- [10] and [01]

**Tetragonal**
- \( a = b \); \( \gamma = 90^\circ \)
- \( \langle 10 \rangle \) ([10] and [01])
- \( \langle 1\bar{1} \rangle \) ([11] and [1\bar{1}])

**Hexagonal**
- \( a = b \); \( \gamma = 120^\circ \)
- \( \langle 10 \rangle \) ([10], [01] and [1\bar{1}])
- \( \langle 1\bar{1} \rangle \) ([21], [12] and [1\bar{1}])

Crystal families: **monoclinic**, **orthorhombic**, **tetragonal**, **hexagonal**
Type of lattice*: **primitive**, **centred**

*Lattice whose conventional unit cell is primitive or centred
Direction indices $[uv]$ in the hexagonal lattice of $E^2$
Why not 5, then?
The concept of holohedry

Symmetry of the lattice: $S_L = 4mm$

Symmetry of the object: $S_o = 4mm$

Symmetry of the pattern: $S_p = 4mm$

$Lattice$

«Object» (content of the unit cell)

Pattern

$S_p = S_L : \text{holohedry}$
The concept of merohedry

Symmetry of the lattice: $S_L = 4mm$
Symmetry of the object: $S_o = 3m$
Symmetry of the pattern: $S_p = m = 4mm \cap 3m$

$S_p < S_L$: merohedry
The concept of merohedry

Symmetry of the lattice : $S_L = 4mm$

Symmetry of the object : $S_o = 3m$

Symmetry of the pattern : $S_p = 1 = 4mm \cap 3m$

$S_p < S_L : \text{merohedry}$
The concept of merohedry

The crystallographic restriction \((n = 1, 2, 3, 4, 6)\) applies to the lattice and to the pattern, but not to the content of the unit cell!

Symmetry of the lattice : \(S_L = 4mm\)

Symmetry of the object : \(S_o = 5m\)

Symmetry of the pattern : \(S_p = m = 4mm \cap 5m\)

\(S_p < S_L\) : merohedry
The inversion – an operation that exists only in odd-dimensional spaces

Inversion centre (point)

Why?
Matrix representation of the inversion in $E^n$

\[
\begin{pmatrix}
\bar{1} & \bar{1} & \cdots & \bar{1} \\
\bar{1} & \bar{1} & \cdots & \bar{1} \\
\bar{1} & \bar{1} & \cdots & \bar{1} \\
\end{pmatrix}
\begin{pmatrix}
x \\
y \\
z \\
w \\
\end{pmatrix}
= \begin{pmatrix}
-x \\
-y \\
-z \\
-w \\
\end{pmatrix}
\]

\[
\bar{1} = -I^n
\]

\[
\text{det}(\bar{1}) = (-1)^n
\]

Example in $E^2$

\[
\begin{pmatrix}
1 & 2 \\
4 & 3 \\
\end{pmatrix}
\xrightarrow{\text{"\bar{1}" operation}}
\begin{pmatrix}
3 & 4 \\
2 & 1 \\
\end{pmatrix}
\]

Two-fold rotation!
Symmetry in three dimensions
(E³ : the three-dimensional Euclidean space)

Operations that leave invariant all the space (3D): the identity
Operations that leave invariant a plane (2D): the reflections
Operations that leave invariant one direction of the space (1D): the rotations
Operations that leave invariant one point of the space (0D): the roto-inversions
Operations that do not leave invariant any point of the space: the translations

The subspace left invariant (if any) by the symmetry operation has dimensions from 0 to N (= 3 here)

Three independent directions in E³ ⇒ three axes (a, b, c) and three interaxial angles (α, β, γ)
# Types of symmetry elements and operations in $E^3$ (Hermann-Mauguin symbols)

## Operations of the first kind (no change of chirality)

<table>
<thead>
<tr>
<th>Element</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct axis</td>
<td>Rotation</td>
</tr>
<tr>
<td>1</td>
<td>$2\pi/1$</td>
</tr>
<tr>
<td>2</td>
<td>$2\pi/2$</td>
</tr>
<tr>
<td>3</td>
<td>$2\pi/3$</td>
</tr>
<tr>
<td>4</td>
<td>$2\pi/4$</td>
</tr>
<tr>
<td>6</td>
<td>$2\pi/6$</td>
</tr>
</tbody>
</table>

## Operations of the second kind (change of chirality)

<table>
<thead>
<tr>
<th>Element</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inverse axis</td>
<td>Rotoinversion</td>
</tr>
<tr>
<td>$\overline{1}$ (centre)</td>
<td>inversion</td>
</tr>
<tr>
<td>$\overline{2}$ ($m$)</td>
<td>reflexion</td>
</tr>
<tr>
<td>$\overline{3}$</td>
<td>$2\pi/3 +$ inversion</td>
</tr>
<tr>
<td>$\overline{4}$</td>
<td>$2\pi/4 +$ inversion</td>
</tr>
<tr>
<td>$\overline{6}$</td>
<td>$2\pi/6 +$ inversion</td>
</tr>
</tbody>
</table>

Operations resulting from a combination with a translation are introduced later.

The orientation in space of a rotation axis or mirror plane is always expressed with respect to the lattice direction to which these are parallel or perpendicular respectively.
Labelling of axes and angles in $\mathbb{E}^3$
Equivalence of $\bar{2}$ and $m$
Combination of 2 and 1 gives \( m \)

Applies to even-fold rotations as well, because they all “contain” a twofold rotation.
Types of unit cells in $E^3$

The unit cell of type $R$ is defined later.
Crystal families and types of lattices in $E^3$: the triclinic (anorthic) family

- A third direction inclined to the plane $\Rightarrow$ the rotation points in each 2D lattice do not overlap to form a rotation axis in the 3D lattice.

- 2D $\rightarrow$ 3D

- $2 \otimes \bar{1} = \bar{1}$

- Triclinic crystal family (anorthic)
  - One symmetry element: the inversion centre
  - No symmetry direction
  - The conventional unit cell is not defined $-$ no reason to choose $\text{à priori}$ a centred cell
  - Symmetry of the lattice: $\bar{1}$
  - No restriction on $a$, $b$, $c$, $\alpha$, $\beta$, $\gamma$
Crystal families and types of lattices in $\mathbb{E}^3$: the monoclinic family

+ a third direction **perpendicular** to the plane $\Rightarrow$ the rotation **points** in each 2D lattice **do** overlap to form a rotation axis in the 3D lattice.

$$2 \rightarrow 2 \otimes \bar{1} = 2/m$$

**Monoclinic crystal family**

- One symmetry direction (**usually** taken as the $b$ axis).
- The conventional unit cell has two right angles ($\alpha$ and $\gamma$).
- Symmetry of the lattice: $2/m$
- Two independent types of unit cell respect these conditions
A lattice of type $mP$ is equivalent to $mB$ but not to $mC$.

Show that unit cells of type $mC$ and $mP$ do not represent the same type of lattice.
Lattices of type $mC$, $mA$, $mI$ and $mF$ are all equivalent ($mS$)
### Three monoclinic settings

<table>
<thead>
<tr>
<th>Setting</th>
<th>$b$-unique</th>
<th>$c$-unique</th>
<th>$a$-unique</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\beta$ unrestricted by symmetry</td>
<td>$\gamma$ unrestricted by symmetry</td>
<td>$\alpha$ unrestricted by symmetry</td>
</tr>
</tbody>
</table>

- $mB = mP$
- $mA = mC = mI = mF$
- $mC = mP$
- $mA = mB = mI = mF$
- $mA = mP$
- $mB = mC = mI = mF$
- $mB = mC = mI = mF$

The symbol of a monoclinic space group will change depending on which setting and what type of unit cell you choose, leading to up to 21 possible symbols for a monoclinic space group.
Crystal families and types of lattices in $E^3$: the orthorhombic family

- Three symmetry directions (axes $a, b, c$)
- The conventional unit cell has three right angles ($\alpha, \beta, \gamma$)
- Symmetry of the lattice: $2/m 2/m 2/m$
- Four types of cell respect these conditions
- The unit cell with one pair of faces centred can be equivalently described as $A, B$ or $C$ by a permutation of the (collective symbol: $S$)

+ a third direction perpendicular to the plane

**orthorhombic crystal family**

$2mm \xrightarrow{\otimes \overline{1}} 2/m2/m2/m$
Three possible setting for the oS type of lattice in $E^3$
Crystal families and types of lattices in $\mathbb{E}^3$: the tetragonal family

- Five symmetry directions ($c, a \& b$, the two diagonals in the $a-b$ plane)
- Symmetry of the lattice: $4/m \ 2/m \ 2/m$
- The conventional cell has three right angles and two identical edges
- Two independent types of unit cell respect these conditions: $tP$ (equivalent to $tC$) and $tI$ (equivalent to $tF$)

+ a third direction perpendicular to the plane

$\text{tetragonal crystal family}$

- $2D \rightarrow 3D$
- $4mm \rightarrow 4mm \otimes \bar{1} = 4/m2/m2/m$
Why unit cells of type \( tA \) et \( tB \) cannot exist?

4-fold axis!
Why unit cells of type \( tA \) et \( tB \) cannot exist?
Why unit cells of type $tA$ et $tB$ cannot exist?
Why unit cells of type \( tA \) et \( tB \) cannot exist?
Why unit cells of type $tA$ et $tB$ cannot exist?

$tF! \rightarrow tI!$
Crystal families and types of lattices in $E^3$: the cubic family

- Thirteen symmetry directions (the 3 axes; the 4 body diagonals; the six face diagonals)
- Symmetry of the lattice: $4/m \overline{3} 2/m$
- The conventional unit cell has three right angles and three identical edges
- Three types of unit cell respect these conditions: $cP$, $cI$ et $cF$

+ a third direction perpendicular to the plane AND $c = a = b$

2D $\rightarrow$ 3D

4$mm$ $\otimes$ $\overline{3}$

= $4/m\overline{3}2/m$

---

**cubic crystal family**
Crystal families and types of lattices in $\mathbb{E}^3$: the hexagonal family

+ a third direction perpendicular to the plane

$6mm \rightarrow 6mm \otimes \overline{1} = 6/m2/m2/m$

**hexagonal crystal family**

+ a new type of unit cell!
Uniqueness of the *hexagonal* crystal family in \( \mathbb{E}^3 \)

\[ A_1, A_2, C \] hexagonal axes parallel to the symmetry directions

\[ a_1, a_2, a_3 \] rhombohedral axes **NOT** parallel to the symmetry directions

**Two types of lattice with different symmetry in the hexagonal crystal family**
Symmetry difference between $hP$ and $hR$ types of lattice

- $6/m2/m2/m$
- $\overline{3}2/m$

- $[\overline{1}10]_H$
- $[\overline{1}01]_R$
- $[\overline{1}20]_H$
- $[120]_H$
- $[010]_H$
- $[0\overline{1}1]_R$
- $[0\overline{1}0]_H$
- $[\overline{1}00]_H$
- $[\overline{1}10]_R$
- $[10\overline{1}]_R$
- $[10\overline{1}]_R$
- $[11\overline{0}]_R$
- $[210]_H$
- $[120]_H$
- $[110]_H$
- $[100]_H$

$\mathbf{\hat{a}}_1$, $\mathbf{\hat{a}}_2$, $\mathbf{\hat{a}}_3$

- $z = 0$
- $z = 1/3$
- $z = 2/3$
Lattice systems: classification based on the symmetry of the lattices

- $\bar{1}$: triclinic
- $2/m$: monoclinic
- $4/m 2/m 2/m$ (4/mmm): tetragonal
- $2/m 2/m 2/m$ (mmm): orthorhombic
- $6/m 2/m 2/m$ (6/mmm): hexagonal
- $\bar{3} m$: rhombohedral
- $4/m \bar{3} m$: cubic
Crystal systems: morphological (macroscopic) and physical symmetry

- Triclinic: $A_1$, 1 or 1
- Monoclinic: $A_2$, 2 or $m$ or $2/m$
- Orthorhombic: $3 \times A_2$, Three twofold elements
- Tetragonal: $A_4$ or $A_3$
- Trigonal: $A_3$, 4 or $A_3$
- Hexagonal: $A_6$
| 6 crystal families | conventional unit cell | 7 crystal systems (morphological symmetry) | 7 lattice systems (lattice symmetry) | 14 types of Bravais lattices

| a = anortic* | no restriction on \( a ; b ; c , \alpha , \beta , \gamma \) | triclinic | triclinic | \( aP \)
| m = monoclinic | no restriction on \( a ; b ; c , \beta . \alpha = \gamma = 90^\circ \) | monoclinic | monoclinic | \( mP (mB) \)
| o = orthorhombic | no restriction on \( a ; b ; c , \alpha = \beta = \gamma = 90^\circ \) | orthorhombic | orthorhombic | \( oP \)
| t = tetragonal | \( a = b ; \alpha = \beta = \gamma = 90^\circ \) aucune restriction sur \( c \) | tetragonal | tetragonal | \( tP (tC) \)
| h = hexagonal | \( a = b ; \alpha = \beta = 90^\circ , \gamma = 120^\circ \) no restriction on \( c \) | trigonal (ternary...)(***) rhombohedral | hexagonal | \( hR \)
| c = cubic | \( a = b = c \) \( \alpha = \beta = \gamma = 90^\circ \) | hexagonal | hexagonal | \( hP \)

(*) Synonyms within parentheses.

(**) \( S = \) one pair of faces centred. Within parentheses the types of lattices that are equivalent (axial setting change – see the monoclinic example).

(***) Crystals of the trigonal crystal system may have a rhombohedral or hexagonal lattice.
Symmetry directions of the lattices in the three-dimensional space (directions in the same box are equivalents by symmetry)

<table>
<thead>
<tr>
<th>Lattice system</th>
<th>Parameters</th>
<th>First symmetry direction</th>
<th>Second symmetry direction</th>
<th>Third symmetry direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>triclinic</td>
<td>$a ; b ; c$</td>
<td>_________________________</td>
<td>_________________________</td>
<td>_________________________</td>
</tr>
<tr>
<td></td>
<td>$\alpha , \beta , \gamma$ any</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>monoclinic</td>
<td>$a ; b ; c$</td>
<td>[010]</td>
<td>_________________________</td>
<td>_________________________</td>
</tr>
<tr>
<td></td>
<td>$\alpha = \gamma = 90^\circ , \beta$ any</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>orthorhombic</td>
<td>$a ; b ; c$</td>
<td>[100]</td>
<td>[010]</td>
<td>[001]</td>
</tr>
<tr>
<td></td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>tetragonal</td>
<td>$a = b ; c$</td>
<td>[001]</td>
<td>[100]</td>
<td>[010]</td>
</tr>
<tr>
<td></td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td></td>
<td>$\equiv \langle 100 \rangle$</td>
<td>$\equiv \langle 1\bar{1}0 \rangle$</td>
</tr>
<tr>
<td>rhombohedral</td>
<td>$a = b = c$</td>
<td>[111]</td>
<td>[1\bar{1}0]</td>
<td>[1\bar{1}0]</td>
</tr>
<tr>
<td></td>
<td>$\alpha = \beta = \gamma$</td>
<td></td>
<td>$\equiv \langle 1\bar{1}0 \rangle$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$a = b ; c$</td>
<td>[001]</td>
<td>[100]</td>
<td>[\bar{1}00]</td>
</tr>
<tr>
<td>rhombohedral</td>
<td>$\alpha = \beta = 90^\circ , \gamma = 120^\circ$</td>
<td></td>
<td>$\equiv \langle 100 \rangle$</td>
<td></td>
</tr>
<tr>
<td>hexagonal</td>
<td>$a = b ; c$</td>
<td>[001]</td>
<td>[100]</td>
<td>[\bar{1}00]</td>
</tr>
<tr>
<td></td>
<td>$\alpha = \beta = 90^\circ , \gamma = 120^\circ$</td>
<td></td>
<td>$\equiv \langle 100 \rangle$</td>
<td>$\equiv \langle 110 \rangle$</td>
</tr>
<tr>
<td>cubic</td>
<td>$a = b = c$</td>
<td>[001]</td>
<td>[100]</td>
<td>[010]</td>
</tr>
<tr>
<td></td>
<td>$\alpha = \beta = \gamma = 90^\circ$</td>
<td></td>
<td>$\equiv \langle 001 \rangle$</td>
<td>$\equiv \langle 111 \rangle$</td>
</tr>
</tbody>
</table>

Massimo Nespolo, Université de Lorraine
## Condition of lattice plane/direction mutual perpendicularity in the seven lattice systems of the three-dimensional space (without metric specialisation)

<table>
<thead>
<tr>
<th>Lattice system</th>
<th>lattice plane</th>
<th>lattice direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>triclinic</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>monoclinic ((b)-unique)</td>
<td>(010)</td>
<td>[010]</td>
</tr>
<tr>
<td>orthorhombic</td>
<td>(100)</td>
<td>[100]</td>
</tr>
<tr>
<td></td>
<td>(010)</td>
<td>[010]</td>
</tr>
<tr>
<td></td>
<td>(001)</td>
<td>[001]</td>
</tr>
<tr>
<td>tetragonal</td>
<td>(001)</td>
<td>[001]</td>
</tr>
<tr>
<td></td>
<td>((hk0))</td>
<td>([hk0])</td>
</tr>
<tr>
<td>rhombohedral and hexagonal</td>
<td>(0001)</td>
<td>[001]</td>
</tr>
<tr>
<td>(hexagonal axes)</td>
<td>((hki0))</td>
<td>([2h+k,h+2k,0])</td>
</tr>
<tr>
<td>Cubic</td>
<td>((hkl))</td>
<td>([hkl])</td>
</tr>
</tbody>
</table>
Point groups and morphological symmetry. Introduction to the stereographic projection

International School on Fundamental Crystallography with applications to Electron Crystallography
June 27 - July 2, 2016 - University of Antwerp
A brief analysis of the symmetry of the square in $E^2$
Find the symmetry elements, the symmetry operations and the symmetry group of a square

Symmetry elements:

- $4$
- $m_{[10]}$
- $m_{[01]}$
- $m_{[11]}$
- $m_{[1\bar{1}]}$

Symmetry operations:

- $4^1$, $4^2=2$, $4^3=4^{-1}$, $4^4=1$
- $m_{[10]}$, $m_{[01]}$, $m_{[11]}$, $m_{[1\bar{1}]}$

Check that the above symmetry operations do form a group

- The identity is included (and obtained as $4^4$ or $m^2$)
- The inverse of each operation is included ($1^{-1}=1$; $m^{-1}=m$; $2^{-1}=2$, $4^{-1}=4^3$)
- For the binary operation and the associativity, build the multiplication table

\[
\begin{array}{c|cc}
\cdot & 1 & 2 & 4 \\
\hline
1 & 1 & 2 & 4 \\
2 & 2 & 4 & 1 \\
4 & 4 & 1 & 2 \\
\end{array}
\]
**Multiplication table of the symmetry operations of a square**

\[
\begin{array}{cccccc}
1 & 2 & 4^1 & 4^3 & m_{[10]} & m_{[11]} \\
2 & 1 & 4^1 & 4^3 & m_{[01]} & m_{[11]} \\
4^1 & 4^1 & 2 & 1 & m_{[11]} & m_{[11]} \\
4^3 & 4^3 & 4^1 & 1 & 2 & m_{[01]} & m_{[10]} & m_{[11]} & m_{[01]} \\
\end{array}
\]

\[
\begin{array}{cccccc}
m_{[10]} & m_{[10]} & m_{[01]} & m_{[11]} & m_{[01]} & m_{[11]} \\
m_{[11]} & m_{[11]} & m_{[10]} & m_{[11]} & m_{[01]} & m_{[10]} \\
m_{[01]} & m_{[01]} & m_{[10]} & m_{[11]} & m_{[11]} & m_{[1T]} & m_{[10]} \\
m_{[1T]} & m_{[1T]} & m_{[11]} & m_{[01]} & m_{[11]} & m_{[10]} & m_{[01]} \\
\end{array}
\]
Subgroups and cosets

A subgroup \((H, \circ)\) of a group \((G, \circ)\) is a subset of the elements of the set \(G\) that under the same binary operation \(\circ\) still forms a group (i.e. it is associative and contains the identity and the inverse of each element).
Subgroups and cosets

A subgroup \((H, \circ)\) of a group \((G, \circ)\) is a subset of the elements of the set \(G\) that under the same binary operation \(\circ\) still forms a group \(i.e.\) it is associative and contains the identity and the inverse of each element.)
Lattice planes and Miller indices
Planes passing through lattice nodes are called “rational planes”

The values $h$, $k$ and $l$ are called the **Miller indices** of the lattice plane and give its orientation. All lattice planes in the same family have the same orientation → $(hkl)$ represents the whole family of lattice planes.

Parametric equation of the plane:

$$\frac{x}{p} + \frac{y}{q} + \frac{z}{r} = 1$$

$$(qr)x + (pr)y + (pq)z = pqr$$

$$hx + ky + lz = m$$

Making $m$ variable, we obtain a family of lattice planes, $(hkl)$, where $h$, $k$ and $l$ are called the Miller indices.

First plane of the family $(hkl)$ for $m = 1$

$$hx + ky + lz = 1$$

Intercepts of the first plane of the family $(hkl)$ on the axes

- $p = \frac{pqr}{qr} = \frac{m}{qr} = \frac{1}{h}$
- $q = \frac{pqr}{pr} = \frac{m}{pr} = \frac{1}{k}$
- $r = \frac{pqr}{pq} = \frac{m}{pq} = \frac{1}{l}$
Why the *reciprocal* of the intersection \((1/p)\) rather than the intersection \((p)\) itself?

Consider a plane parallel to an axis – for example \(c\)

What is the intersection of this plane with the axis \(c\)? \(\infty\)

What is the \(l\) Miller intersection of this plane? \(\frac{1}{\infty} = 0\)
Example: family (112) in a primitive lattice

Intercepts of the first plane of the family:
on $a$: 1/1
on $b$: 1/1
on $c$: 1/2

Intercepts of the second plane of the family:
on $a$: 2/1
on $b$: 2/1
on $c$: 2/2
Example: family (326) in a primitive lattice

Intercepts of the first plane of the family:
on $a$: $\frac{1}{3}$
on $b$: $\frac{1}{2}$
on $c$: $\frac{1}{6}$

Intercepts of the sixth plane of the family:
on $a$: $\frac{6}{3}$
on $b$: $\frac{6}{2}$
on $c$: $\frac{6}{6}$
Miller indices for a primitive lattice are coprime integers

Intercepts of the first plane of a hypothetic family (222):
on $a$: 1/2
on $b$: 1/2
on $c$: 1/2

This plane does not pass through any lattice node – it is an *irrational* plane.

The first rational plane of this family has intercepts:
on $a$: 1/1
on $b$: 1/1
on $c$: 1/1

In a primitive lattice, the Miller indices of a family of lattice planes are coprime integers: (111)
Miller indices for different types of lattice: $(h00)$ in $oP$ and $oC$ (projection on $ab$)

In morphology, we do not see the lattice and thus the Miller indices of a face are usually coprime integers.
The stereographic projection: how to get rid of accidental morphological features of a crystal
Spherical projection and spherical poles
Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')
Building the stereographic projection: from the spherical poles (P) to the stereographic poles (p, p')
Stereographic projection: poles and symmetry planes
Example of decomposition of the morphology of a crystal

Cube

Octahedron

Dodecahedron
Stereographic vs. gnomonic projection

Be careful - some textbooks exchange the two terms!
In case of hexagonal or rhombohedral lattices, it is useful to use a reference built on four axes, three in the plane normal to the unique axis \((\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3)\) and one \((\mathbf{c})\) for the unique axis. Consequently, four indices of lattice planes, \((h k i l)\), are used, called the **Bravais-Miller indices**. Here \(h, k, i, l\) are integers inversely proportional to the intercepts of a plane of the family with the four axes.

Only two of the three axes in a plane are linearly independent: \(\mathbf{A}_3\) is expressed as \(\mathbf{A}_3 = -\mathbf{A}_1 - \mathbf{A}_2\). Analogously, the indices \(h, k, i\) are cyclically permutable and related by \(h + k + i = 0\).
Weber indices

For trigonal and hexagonal crystal, an extension to a four-axes axial setting exists also for lattice directions, known as the **Weber indices**. The Weber indices of the direction perpendicular to a lattice plane are the same as the Bravais-Miller indices of that plane.

Let $A_1, A_2, A_3, C$ be the four hexagonal axes, and let be $uvw$ and $UVTW$ the indices of a direction with respect to $A_1, A_2, C$ or $A_1, A_2, A_3, C$ respectively. The relations between $uvw$ and $UVTW$ are:

$$
u = 2U + V; \quad v = U + 2V; \quad w = W$$

$$U = (2u-v)/3; \quad V = (2v-u)/3; \quad T = -(u+v)/3.$$

The relation $T = -U-V$ holds for $U$ and $V$ but not for $u$ and $v$, whereas for the Bravais-Miller indices the addition of the third axis does not modify $h$ and $k$ so that the relation $i = -h-k$ is applied directly. For this reason, the Bravais-Miller indices are widely used in crystallography, whereas the Weber indices are more used in fields like electron microscopy and metallurgy but seldom in crystallography.

<table>
<thead>
<tr>
<th>Miller indices</th>
<th>Bravais-Miller indices</th>
<th>Perpendicular direction</th>
<th>Perpendicular direction (Weber indices)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(hkl0)</td>
<td>(hki0)</td>
<td>[2h+k,h+2k,0]</td>
<td>[hki0]</td>
</tr>
<tr>
<td>Ex. (100)</td>
<td>(1010)</td>
<td>[210]</td>
<td>[1010]</td>
</tr>
<tr>
<td>Ex. (2T0)</td>
<td>(2T10)</td>
<td>[100]</td>
<td>[2T10]</td>
</tr>
</tbody>
</table>
International School on Fundamental Crystallography with applications to Electron Crystallography

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The concept of form: set of symmetry-related faces

Example in the cubic crystal system

Form \{100\}: the cube

Form \{111\}: the octahedron
Zone: set of faces whose intersection is parallel to a same direction, called the zone axis.

Example in the cubic crystal system

- Zone [001]
- Zone [010]
- Zone [100]
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 \((h\,k\,l)\) if (Weiss law):

\[ u h + v k + w l = 0 \]

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:

\[
\begin{bmatrix}
 u \\
 k_1 & l_1 \\
 k_2 & l_2 \\
\end{bmatrix} = \frac{1}{l_1}
\begin{bmatrix}
 v \\
 k_1 & h_1 \\
 k_2 & h_2 \\
\end{bmatrix} = \frac{1}{h_1}
\begin{bmatrix}
 w \\
 h_1 & k_1 \\
 h_2 & k_2 \\
\end{bmatrix}
\]

Conversely, any crystal face can be determined if one knows two zone axes parallel to it (zone law).

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:

\[
\begin{vmatrix}
 h_1 & k_1 & l_1 \\
 h_2 & k_2 & l_2 \\
 h_3 & k_3 & l_3 \\
\end{vmatrix} = 0
\]
Compute the zone axis

Let the Miller indices of two lattice planes be \((h_1, k_1, l_1), (h_2, k_2, l_2)\).

\[
\begin{array}{c|ccc|c}
  h_1 & k_1 & l_1 & h_1 & l_1 \\
  h_2 & k_2 & l_2 & h_2 & l_2 \\
  \hline
  u & v & w & \text{Remove common factor, if any} \\
\end{array}
\]

Exercise: zone axis for faces (001) and (101)

\[
\begin{array}{cccccc|c}
  0 & 0 & 1 & 0 & 0 & 1 \\
  1 & 0 & 1 & 1 & 0 & 1 \\
  \hline
  0 & 1 & 0 \\
\end{array}
\]

Exercise: zone axis for faces (231) and (362)

\[
\begin{array}{cccccccc|c}
  2 & 3 & 1 & 2 & 3 & 1 \\
  3 & 6 & 2 & 3 & 6 & 2 \\
  \hline
  0 & \bar{1} & 3 \\
\end{array}
\]

Low-index zone axes correspond to lattice rows parallel to several lattice planes

\[
\begin{array}{c|ccc|c}
  h_1 & 0 & l_1 & h_1 & 0 & l_1 \\
  h_2 & 0 & l_2 & h_2 & 0 & l_2 \\
  \hline
  0 & n & 0 & n = l_1h_2 - l_2h_1 \\
\end{array}
\]
Screw axes and glide planes

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Elements and operations

- **geometric element**: the point, line or plane left invariant by the symmetry operation.
- **symmetry element**: the geometric element defined above together with the set of operations (called **element set**) that leave invariant.
- **symmetry operation**: an isometry that leave invariant the object to which it is applied.

The operations that share a given geometric element differ by a lattice vector. The one characterized by the shortest vector is called **defining operation**.
Finding the geometric element

- Remove the intrinsic translation part (screw or glide component).
- Impose that the coordinates of the geometric element are fixed by the operation.

\[
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 1/2 \\
0 & 0 & 1 & 1/2 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

Intrinsic part: screw component

Location part: the element does not pass through the origin

Linear part: twofold rotation about [010]

\[
\begin{pmatrix}
\bar{1} & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 1/2 \\
0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
u \\
v \\
w \\
w
\end{pmatrix}
= 
\begin{pmatrix}
u \\
v \\
w \\
w
\end{pmatrix}
\]

\[
\begin{cases}
-u = u \\
v = v \\
-w + 1/2 = w
\end{cases}
\]

\[
\begin{cases}
u = 0 \\
\forall v \\
0, y, 1/4
\end{cases}
\]
Screw axes $n_p$ (screw component: $p/n$)

**Geometric element**: line

**Defining operation**: twofold screw rotation

**Symmetry element**: screw axis

---

**Defining operation**: twofold rotation

**Symmetry element**: rotation axis

---

Period

Half period
Glide planes $g$

Geometric element: plane

Special cases:
- $g\ (0,0,0): m$
- $g\ (0,\frac{1}{2},0): b$
- $g\ (\text{half-diagonal}): n$
- $g\ (\frac{1}{2},0,0): a$
- $g\ (0,0,\frac{1}{2}): c$
- $g\ (\text{quarter-diagonal}): d$
Screw axes

2

\[
\begin{array}{c}
0 \\
0
\end{array}
\]

1/2

\[
\begin{array}{c}
1/2 \\
0
\end{array}
\]

2/3

\[
\begin{array}{c}
1/3 \\
2/3
\end{array}
\]

3/2

\[
\begin{array}{c}
1/3 \\
2/3
\end{array}
\]
Screw axes

$4$

$4_1$

$4_2 \supset 2$

$4_3$

$\frac{1}{4}$

$\frac{1}{2}$

$\frac{3}{4}$

$\frac{1}{2}$

$0$

$0$

$0$

$0$

$0$
Screw axes
Screw axes

\[ n_p \]

\[ n_{n-p} \]
Glide planes
Glide planes
Glide planes

Diamond structure glide plane

2D glide line; 3D glide plane with “unusual' glide
Glide planes

d/2

\[ \text{e} \]

\[ \text{g} \]
How can we have a glide of $\frac{1}{4}$ if the reflection is an operation of order 2?

If the unit cell is centred!

Vector centring the unit cell, with a norm $d/2$
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Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

Auguste Bravais (1811-1863)
Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

\[ a \times b = S(001) \]

\[ e_{(001)} = \frac{a \times b}{|a \times b|} \]

\[ V = c \cdot a \times b = S(001)d_{(001)} = S(hkl)d_{(hkl)} \]
Bravais' polar lattice (1848)
A dual lattice of the direct lattice based on face normals

The vector space $V^n$ is realized with a metric in Å obeying the above conditions

$|r^p_{hkl}| = S(hkl)/V^{1/3} = [V/d_{(hkl)}]/V^{1/3} = V^{2/3}/d_{(hkl)}$ (Å)
By construction, the vector $[hkl]^p$ is perpendicular to the face $(hkl)$. 

\[ a^p = \frac{S(100)}{V^{1/3}} = \frac{b \times c}{V^{1/3}}; \quad b^p = \frac{S(010)}{V^{1/3}} = \frac{c \times a}{V^{1/3}}; \quad a^p = \frac{S(001)}{V^{1/3}} = \frac{a \times b}{V^{1/3}} \]
Angles between vectors of the polar lattice are precisely the angles between face normals.

\[ \delta = \pi - \varphi \]

\[ \cos \delta = \frac{r_1^p \cdot r_2^p}{||r_1^p|| \cdot ||r_2^p||} = \frac{\begin{pmatrix} h_1 \\ k_1 \\ l_1 \end{pmatrix}_{\text{G}^p} \begin{pmatrix} h_2 \\ k_2 \\ l_2 \end{pmatrix}}{\begin{pmatrix} h_1 \\ k_1 \\ l_1 \end{pmatrix}_{\text{G}^p} \begin{pmatrix} h_1 \\ k_1 \\ l_1 \end{pmatrix}_{\text{G}^p} \begin{pmatrix} h_2 \\ k_2 \\ l_2 \end{pmatrix}_{\text{G}^p}} \]

\[ G^p = \begin{pmatrix} a^p \cdot a^p \\ a^p \cdot b^p \\ a^p \cdot c^p \\ b^p \cdot a^p \\ b^p \cdot b^p \\ b^p \cdot c^p \\ c^p \cdot a^p \\ c^p \cdot b^p \\ c^p \cdot c^p \end{pmatrix} \]
Use of the polar lattice makes indexing of stereographic poles straightforward – monoclinic example

- Parallel to $a$ and $b$ axes on the $c^p$ axis
- Parallel to $c$ and $b$ axes on the $a^p$ axis
- (001)
- (100)
Use of the polar lattice makes indexing of stereographic poles straightforward – hexagonal example

Parallel to $A_2$ and $C$ axes

On the $a^p$ axis

Same intersection on $A_1$ and $A_2$ (positive)
Half intersection on $A_3$ (negative)

On the bisector of $a^p$ and $b^p$
Use of the polar lattice makes indexing of stereographic poles straightforward – hexagonal example
Then, something happened....

Wilhelm Conrad Röntgen
(1845-1923)
1895 : discovery of X-rays
1912: crystals diffract X-rays

Max von Laue  
(1879-1960)
1912: crystals diffract X-rays

X-ray diffraction pattern of ZnS by Friedrich, Knipping and Laue
A diffraction pattern can be indexed with a lattice whose metric is inverse (reciprocal) of the Bravais lattices.
1913: the reciprocal lattice

Paul Peter Ewald (1888-1985)
The reciprocal lattice

The reciprocal space is a vector space $V^n$ realized with a metric in Å$^{-1}$.
Linear parameters of the reciprocal lattice

\[ a^* = (b \times c)/V, \quad b^* = (c \times a)/V, \quad c^* = (a \times b)/V \]

\[ a^* = bcsin\alpha/V, \quad b^* = casin\beta/V, \quad c^* = absin\gamma/V \]

\[ a \cdot a^* = a \cdot (b \times c)/V = 1; \quad b \cdot b^* = b \cdot (c \times a)/V = 1; \quad c \cdot c^* = c \cdot (a \times b)/V = 1 \]

\[ \mathbf{v}_i \cdot \mathbf{v}_j^* = \delta_{ij} \]

\[ V^* = a^* \cdot b^* \times c^* = (b \times c) \cdot (c \times a) \times (a \times b)/V^3 = (b \times c) \cdot [(c \cdot a \times b)a-(c \cdot a \times a)b]/V^3 = \]

\[ (b \times c) \cdot [Va-0b]/V^3 = V^2/V^3 = 1/V \]

\[ a = (b^* \times c^*)/V^*; \quad b = (c^* \times a^*)/V^*; \quad c = (a^* \times b^*)/V^* \]
Angular parameters of the reciprocal lattice

\[ a^* = bc \sin \alpha / V, \quad b^* = ca \sin \beta / V, \quad c^* = ab \sin \gamma / V \]

\[ a = b^* c^* \sin \alpha^*/V^*; \quad b^* = a^* c^* \sin \beta^*/V^*; \quad c^* = a^* b^* \sin \gamma^*/V^* \quad (V^* = 1/V) \]

\[ \sin \alpha^* = \frac{a V^*}{b^* c^*} = \frac{a V}{ac \sin \beta \, ab \sin \gamma \, V} = \frac{V}{abc \sin \beta \sin \gamma} \]

\[ \sin \beta^* = \frac{b V^*}{a^* c^*} = \frac{b V}{bc \sin \alpha \, ab \sin \gamma \, V} = \frac{V}{abc \sin \alpha \sin \gamma} \]

\[ \sin \gamma^* = \frac{c V^*}{a^* b^*} = \frac{c V}{bc \sin \alpha \, ac \sin \beta \, V} = \frac{V}{abc \sin \alpha \sin \beta} \]
Metric tensor of the reciprocal lattice

\[
G^* = \begin{bmatrix}
a^* \cdot a^* & a^* \cdot b^* & a^* \cdot c^* \\
b^* \cdot a^* & b^* \cdot b^* & b^* \cdot c^* \\
c^* \cdot a^* & c^* \cdot b^* & c^* \cdot c^*
\end{bmatrix}
\]

\[G^* = G^{-1}; \quad \text{det}(G^*) = 1/\text{det}(G) \implies V^* = 1/V\]

Angles between the \((h_1k_1l_1)\) and \((h_2k_2l_2)\) faces computed as angle between \(r^*(h_1k_1l_1)\) and \(r^*(h_2k_2l_2)\) vectors

\[
\cos(\theta) = \frac{\langle h_1 \ k_1 \ l_1 | G^* | h_2 \ k_2 \ l_2 \rangle}{\sqrt{\langle h_1 \ k_1 \ l_1 | G^* | h_1 \ k_1 \ l_1 \rangle} \sqrt{\langle h_2 \ k_2 \ l_2 | G^* | h_2 \ k_2 \ l_2 \rangle}}
\]
Equidistance of lattice planes

\[ d_{(hkl)} = \frac{a}{h} \cdot \frac{h a^* + k b^* + l c^*}{|r_{hkl}^*|} = \frac{h 1 + k 0^* + l 0}{h |r_{hkl}^*|} = \frac{1}{r_{hkl}^*} \]

\[ d_{(hkl)} = \frac{b}{k} \cdot \frac{h a^* + k b^* + l c^*}{|r_{hkl}^*|} = \frac{h 0 + k 1^* + l 0}{k |r_{hkl}^*|} = \frac{1}{r_{hkl}^*} \]

\[ d_{(hkl)} = \frac{c}{l} \cdot \frac{h a^* + k b^* + l c^*}{|r_{hkl}^*|} = \frac{h 0 + k 0^* + l 1}{l |r_{hkl}^*|} = \frac{1}{r_{hkl}^*} \]
Not really Ewald's discovery....

Reciprocal system of vectors (1881)

Josiah Willard Gibbs
(1839-1903)
VECTOR ANALYSIS

A TEXT-BOOK FOR THE USE OF STUDENTS
OF MATHEMATICS AND PHYSICS

FOUNDED UPON THE LECTURES OF

J. WILLARD GIBBS, Ph.D., LL.D.
Formerly Professor of Mathematical Physics in Yale University

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Vector Analysis

A Text-Book for the Use of Students of Mathematics and Physics, Founded Upon the Lectures of J. Willard Gibbs.

J. Willard Gibbs

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Geometric interpretation of reflection conditions

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Classification of reflection conditions

- **General**: apply to all Wyckoff positions.
- **Special**: apply to special Wyckoff positions. In particular, in presence of non-characteristic and extraordinary orbits one gets additional special reflection conditions.
- **Integral**: appear when a non-primitive unit cell is selected.
- **Zonal**: appear in presence of glide planes.
- **Serial**: appear in presence of screw axes.

**Warning!**

- Systematic extinctions
- Systematic absences (actually, presences!)

Reflection conditions
When you choose a primitive unit cell you do not see integral reflection conditions.

Integral reflection condition: depend on the choice of the unit cell, not on the structure.

**C-centred unit cell**

\( hkl : h + k = 2n \)

**Primitive unit cell**

No conditions

**When you choose a primitive unit cell you do not see integral reflection conditions**
Zonal reflection conditions: witness of glide planes
Zonal reflection conditions: witness of glide planes

**Direct space**
In projection along the **a** axis the period along **b** seems halved

**Reciprocal space**
On the (0kl)*plane the period along the **b*** axis appears doubled.

**Reflection conditions**: \(0kl : k = 2n\)
Serial reflection conditions: witness of screw axes

**Direct space**
In the projection on the $c$ axis the period appears reduced to $\frac{1}{4}$.

**Reciprocal space**
In the [001]* direction the period appears multiplied by four.

Reflection conditions:
$00l : l = 4n$
From reflections conditions to space groups
Example 1: orthorhombic

Integral reflection conditions: centred cell

\[ hkl: k + l = 2n \]
\[ 0kl: k + l = 2n \]
\[ h0l: l = 2n \]
\[ h00: h = 2n \]
\[ hk0: h = 2n \]
\[ hk0: k = 2n \]
\[ h00: h = 2n \]
\[ 0k0: k = 2n \]
\[ 00l: l = 2n \]

Zonal reflection conditions: glide plane

Extension symbol: \( A--a \)

Possible space-group types: \( Am2a, A2_1ma, Amma \)
Exemple 2: tetragonal

No integral reflection condition $\rightarrow tP$

\[ \begin{align*}
    h0k0: & h+k = 2n \\
    0k0: & k = 2n \\
    hhl: & l = 2n \\
    00l: & l = 2n
\end{align*} \]

Zonal reflection conditions: glide plane

Zonal reflection conditions: glide plane

Non-independent

Extinction symbol: $Pn\text{-}c$

Possible space-group type: $P4_2/nmc$
Example 3: cubic

- **hkl**: $h+k+l = 2n$
  - Integral reflection condition
  - **0kl**: $k = 2n$
  - **0kl**: $l = 2n$
  - **h0l**: $h = 2n$
  - **h0l**: $l = 2n$
  - **hk0**: $h = 2n$
  - **hk0**: $k = 2n$
  - **hhl**: $2h+l = 4n$
  - **hhl**: $l = 2n$
  - **00l**: $l = 4n$

- Zonal reflection condition

- **0kl**: perpendicular to [100], $k$ even
  - **0kl**: perpendicular to [001], $l$ even
  - **h0l**: perpendicular to [010], $h$ even
  - **h0l**: perpendicular to [010], $l$ even
  - **hk0**: perpendicular to [001], $h$ even
  - **hk0**: perpendicular to [001], $k$ even
  - **hhl**: perpendicular to [110], $2h+l = 4n$
Direct lattice: \((a+b+c)/4\)  
Reciprocal lattice: \(h+k+l = 4n\)  
\[ (110) \Rightarrow h = k \quad h+h+l = 4n \]

\[ hhl:2h+l = 4n \]  
\[ d_{[1\bar{1}0]} \]
Example 3: cubic

Extinction symbol: $Ia-d$

Possible space-group type: $Ia\overline{3}d$
Reflection conditions

$h, k, l$ permutably
General:

\[hkl : h + k + l = 2n\]
\[0kl : k, l = 2n\]
\[hhl : 2h + l = 4n\]
\[h00 : h = 4n\]
Hierarchy of classification
Point group

$mmm$

Symmorphic space group

$Pmmm$

site-symmetry group at the origin: $mmm$

Hemisymmorphic space group

$Pnnn$

s.-s. group at the origin: 222

Asymmorphic space group

$Pmna$

s.-s. group at the origin: $2/m$

Asymmorphic space group

$Pcca$

s.-s. group at the origin: $\overline{1}$
A geometric crystal class which represents a full symmetry of a lattice is called a **holohedry**. Otherwise, a **merohedry**.
Crystal systems
Space groups and crystal structures whose point group act of the same type of Bravais lattice belong to the same crystal system.

\[ H, G: \text{point groups} \quad H \subset G \]

If \( G \) acts on lattice, then \( H \) to acts on the same lattice

If \( H \) acts on lattice, \( G \) does not necessarily act on the same lattice

Ex. 1: \( \overline{m} \overline{3}m \) (\( G \)) acts on \( cP, cI, cF \). 23, \( m3, 432, \overline{43}m \) (\( H \)) act on the same lattices

\( 23 \) (\( H \)) acts on \( cP, cI, cF. \overline{m} \overline{3}m \) (\( G \)) act on the same lattices. Etc.

Crystals with point groups \( \overline{m} \overline{3}m, m3, 432, \overline{43}m, 23 \) all belong to the cubic crystal system.

Ex. 2: \( 6/m \overline{m} \overline{m} \) (\( G \)) acts on \( hP. 6, \overline{6}, 6/m, 622, 6\overline{m}, \overline{6}2m, 3, \overline{3}, 32, 3m, \overline{3}m \) (\( H \)) act on \( hP \) too.

\( \overline{3}m \) (\( H \)) acts on \( hP \) and \( hR \) but \( 6/m \overline{m} \overline{m} \) (\( G \)) does not act on \( hR \).

\( 6 \) (\( H \)) acts on \( hP. 6/m \overline{m} \overline{m} \) (\( G \)) acts on \( hP \) too.

Crystals with point groups \( 6/m \overline{m} \overline{m}, 6, \overline{6}, 6/m, 622, 6\overline{m}, \overline{6}2m \) all belong to the hexagonal crystal system. Those with point groups \( 3, 3, 32, 3m, \overline{3}m \) belong to the trigonal crystal system.
Lattice systems
Space groups and crystal structures which correspond to the same holohedry belong to the same lattice system.

Ex. 1: $23P$ and $m3P$ correspond to the $m\bar{3}m$ holohedry and belong to the cubic lattice system.

Ex. 2: $32P$ and $622P$ correspond to the $6/mmm$ holohedry and belong to the hexagonal lattice system.

Ex. 3: $32R$ and $622P$ correspond to the different holohedries ($\bar{3}m$ and $6/mmm$). $32R$ belong to the rhombohedral lattice system, whereas $622$ belongs to the hexagonal lattice system.
Crystal families
Space groups and crystal structures whose lattices have the same number of free parameters belong to the same crystal family if the corresponding point groups are in group-subgroup relation.

Ex. 1: Two crystals with holohedries $4/mmm$ and $6/mmm$ have lattices with two free parameters ($a$ and $c$). However, $4/mmm$ and $6/mmm$ are not in group-subgroup relation and thus the two crystals belong to different crystal families (tetragonal and hexagonal).

Ex. 2: Two crystals with holohedries $\overline{3}m$ and $6/mmm$ have lattices with two free parameters ($a$ and $c$). Furthermore, $\overline{3}m$ is a subgroup of $6/mmm$ and thus the two crystals belong to the same crystal family (hexagonal).
Bravais flocks
Point group order
Point group order